

Minimization of the Energy of the Non-Relativistic One-Electron Pauli-Fierz Model over Quasifree States

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December 11, 2013

Abstract

In this article is proved the existence and uniqueness of a minimizer of the energy for the non-relativistic one electron Pauli-Fierz model, within the class of pure quasifree states. The minimum of the energy on pure quasifree states coincides with the minimum of the energy on quasifree states. Infrared and ultraviolet cutoffs are assumed, along with sufficiently small coupling constant and momentum of the dressed electron. A perturbative expression of the minimum of the energy on quasifree states for a small momentum of the dressed electron and small coupling constant is then given. We also express the Lagrange equation for the minimizer, in terms of the generalized one particle density matrix of the pure quasifree state.

I Introduction

I.1 The Hamiltonian

According to the *Standard Model of Nonrelativistic Quantum Electrodynamics* [2] the unitary time evolution of a free nonrelativistic particle coupled to the quantized radiation field is generated by the Hamiltonian

$$\tilde{H}_g := \frac{1}{2} \left(\frac{1}{i} \vec{\nabla}_x - \vec{A}(\vec{x}) \right)^2 + H_f \quad (\text{I.1})$$

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acting on the Hilbert space $L^2(\mathbb{R}_x^3; \mathfrak{F})$ of square-integrable functions with values in the photon Fock space

$$\mathfrak{F} := \mathfrak{F}_+(\mathcal{Z}) := \bigoplus_{n=0}^{\infty} \mathfrak{F}_+^{(n)}(\mathcal{Z}), \quad (\text{I.2})$$

where $\mathfrak{F}_+^{(0)}(\mathcal{Z}) = \mathbb{C} \cdot \Omega$ is the vacuum sector and the n -photon sector $\mathfrak{F}_+^{(n)}(\mathcal{Z}) = \mathcal{S}(\mathcal{Z}^{\otimes n})$ is the subspace of totally symmetric vectors on the n -fold tensor product of the one-photon Hilbert space

$$\mathcal{Z} = \{ \vec{f} \in L^2(S_{\sigma,\Lambda}; \mathbb{C} \otimes \mathbb{R}^3) \mid \forall \vec{k} \in S_{\sigma,\Lambda} \text{ a.e. : } \vec{k} \cdot \vec{f}(\vec{k}) = 0 \} \quad (\text{I.3})$$

of square-integrable, transversal vector fields which are supported in the momentum shell

$$S_{\sigma,\Lambda} := \{ \vec{k} \in \mathbb{R}^3 \mid \sigma \leq |\vec{k}| \leq \Lambda \}, \quad (\text{I.4})$$

where $0 \leq \sigma < \Lambda < \infty$ are infrared and ultraviolet cutoffs, respectively, reflecting our choice of gauge, namely, the Coulomb gauge. It is convenient to fix real polarization vectors $\vec{\varepsilon}_{\pm}(\vec{k}) \in \mathbb{R}^3$ such that $\{ \vec{\varepsilon}_+(\vec{k}), \vec{\varepsilon}_-(\vec{k}), \frac{\vec{k}}{|\vec{k}|} \} \subseteq \mathbb{R}^3$ form a right-handed orthonormal basis (Dreibein) and replace (I.3) by

$$\mathcal{Z} = L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2), \quad (\text{I.5})$$

with the understanding that $\vec{f}(\vec{k}) = \vec{\varepsilon}_+ f(\vec{k}, +) + \vec{\varepsilon}_- f(\vec{k}, -)$.

In (I.1) the energy of the photon field is represented by

$$H_f = \int |k| a^*(k) a(k) dk, \quad (\text{I.6})$$

where $\int f(k) dk := \sum_{\tau=\pm} \int_{S_{\sigma,\Lambda}} f(\vec{k}, \tau) d^3k$ and $\{a(k), a^*(k)\}_{k \in S_{\sigma,\Lambda} \times \mathbb{Z}_2}$ are the usual boson creation and annihilation operators constituting a Fock representation of the CCR on \mathfrak{F} , i.e.,

$$[a(k), a(k')] = [a^*(k), a^*(k')] = 0, \quad (\text{I.7})$$

$$[a(k), a^*(k')] = \delta(k - k') \mathbf{1}, \quad a(k)\Omega = 0, \quad (\text{I.8})$$

for all $k, k' \in S_{\sigma,\Lambda} \times \mathbb{Z}_2$. The magnetic vector potential $\vec{A}(\vec{x})$ is given by

$$\vec{A}(\vec{x}) = \int \vec{G}(k) \left(e^{-i\vec{k} \cdot \vec{x}} a^*(k) + e^{i\vec{k} \cdot \vec{x}} a(k) \right) dk, \quad (\text{I.9})$$

with $k = (\vec{k}, \tau) \in \mathbb{R}^3 \times \mathbb{Z}_2$,

$$\vec{G}(\vec{k}, \tau) := g \vec{\varepsilon}_\tau(\vec{k}) |\vec{k}|^{-1/2}, \quad (\text{I.10})$$

and $g \in \mathbb{R}$ being the coupling constant. In our units, the mass of the particle and the speed of light equal one, so the coupling constant is given as $g = \frac{1}{4\pi} \sqrt{\alpha}$, with $\alpha \approx 1/137$ being Sommerfeld's fine structure constant.

The Hamiltonian \tilde{H}_g preserves (i.e., commutes with) the total momentum operator $\vec{p} = \frac{1}{i} \vec{\nabla}_x + \vec{P}_f$ of the system, where

$$\vec{P}_f = \int \vec{k} a^*(k) a(k) dk \quad (\text{I.11})$$

is the photon field momentum. This fact allows us to eliminate the particle degree of freedom. More specifically, introducing the unitary

$$\mathbb{U} : L^2(\mathbb{R}_x^3; \mathfrak{F}) \rightarrow L^2(\mathbb{R}_p^3; \mathfrak{F}), \quad (\mathbb{U}\Psi)(\vec{p}) := \int e^{-i\vec{x} \cdot (\vec{p} - \vec{P}_f)} \Psi(\vec{x}) \frac{d^3x}{(2\pi)^{3/2}}, \quad (\text{I.12})$$

one finds that

$$\mathbb{U} \tilde{H}_g \mathbb{U}^* = \int^\oplus H_{g, \vec{p}} d^3p, \quad (\text{I.13})$$

where

$$H_{g, \vec{p}} = \frac{1}{2} (\vec{P}_f + \mathbb{A}(\vec{0}) - \vec{p})^2 + H_f \quad (\text{I.14})$$

is a selfadjoint operator on $\text{dom}(H_{0, \vec{0}})$, the natural domain of $H_{0, \vec{0}} = \frac{1}{2} \vec{P}_f^2 + H_f$.

I.2 Ground State Energy

Due to (I.13), all spectral properties of \tilde{H}_g are obtained from those of $\{H_{g, \vec{p}}\}_{\vec{p} \in \mathbb{R}^3}$. Of particular physical interest is the mass shell for fixed total momentum $\vec{p} \in \mathbb{R}^3$, coupling constant $g \geq 0$, and infrared and ultraviolet cutoffs $0 \leq \sigma < \Lambda < \infty$, i.e., the value of the ground state energy

$$E_{\text{gs}}(g, \vec{p}, \sigma, \Lambda) := \inf \sigma[H_{g, \vec{p}}] \geq 0 \quad (\text{I.15})$$

and the corresponding ground states (or approximate ground states).

We express the ground state energy in terms of density matrices with finite energy expectation value and accordingly introduce

$$\widetilde{\mathfrak{M}} := \left\{ \rho \in \mathcal{L}^1(\mathfrak{F}) \mid \rho \geq 0, \text{Tr}_{\mathfrak{F}}[\rho] = 1, \rho H_{0, \vec{0}}, H_{0, \vec{0}} \rho \in \mathcal{L}^1(\mathfrak{F}) \right\}, \quad (\text{I.16})$$

so that the Rayleigh-Ritz principle appears in the form

$$E_{\text{gs}}(g, \vec{p}) = \inf \left\{ \text{Tr}_{\mathfrak{F}}[\rho H_{g, \vec{p}}] \mid \rho \in \widetilde{\mathfrak{DM}} \right\}. \quad (\text{I.17})$$

Note that $\text{Tr}_{\mathfrak{F}}[\rho H_{g, \vec{p}}] = \text{Tr}_{\mathfrak{F}}[\rho^{1-\beta} H_{g, \vec{p}} \rho^{\beta}]$, for all $0 \leq \beta \leq 1$, due to our assumption $\rho H_{0, \vec{0}}, H_{0, \vec{0}} \rho \in \mathcal{L}^1(\mathfrak{F})$.

It is not difficult to see that the ground state energy is already obtained as an infimum over all density matrices

$$\mathfrak{DM} := \left\{ \rho \in \widetilde{\mathfrak{DM}} \mid \rho N_f, N_f \rho \in \mathcal{L}^1(\mathfrak{F}) \right\} \quad (\text{I.18})$$

of finite photon number expectation value, where

$$N_f = \int a^*(k) a(k) dk \quad (\text{I.19})$$

is the photon number operator. Indeed, if $\sigma > 0$ then

$$H_{g, \vec{p}} \geq H_f \geq \sigma N_f, \quad (\text{I.20})$$

and $\mathfrak{DM} = \widetilde{\mathfrak{DM}}$ is automatic. Furthermore, if $\sigma = 0$ then it is not hard to see [2] that $E_{\text{gs}}(g, \vec{p}, 0, \Lambda) = \lim_{\sigma \searrow 0} E_{\text{gs}}(g, \vec{p}, \sigma, \Lambda)$, by using the standard relative bound

$$\|\vec{\mathbb{A}}_{<\sigma}(\vec{0}) \psi\| \leq \mathcal{O}(\sigma) \|(H_{f, <\sigma} + 1)^{1/2} \psi\|, \quad (\text{I.21})$$

where $\vec{\mathbb{A}}_{<\sigma}(\vec{0})$ and $H_{f, <\sigma}$ are the quantized magnetic vector potential and field energy, respectively, for momenta below σ . So, for all $0 \leq \sigma < \Lambda < \infty$, we have that

$$E_{\text{gs}}(g, \vec{p}, \sigma, \Lambda) = \inf \left\{ \text{Tr}_{\mathfrak{F}}[\rho H_{g, \vec{p}}(\sigma, \Lambda)] \mid \rho \in \mathfrak{DM} \right\}, \quad (\text{I.22})$$

indeed. If the infimum (I.22) is attained at $\rho_{\text{gs}}(g, \vec{p}, \sigma, \Lambda) \in \mathfrak{DM}$ then we call $\rho_{\text{gs}}(g, \vec{p}, \sigma, \Lambda)$ a ground state of $H_{g, \vec{p}}(\sigma, \Lambda)$.

Since \mathfrak{DM} is convex, we may restrict the density matrices in (I.22) to vary only over pure density matrices,

$$E_{\text{gs}}(g, \vec{p}, \sigma, \Lambda) = \inf \left\{ \text{Tr}_{\mathfrak{F}}[\rho H_{g, \vec{p}}(\sigma, \Lambda)] \mid \rho \in \mathfrak{pDM} \right\}, \quad (\text{I.23})$$

where *pure* density matrices are those of rank one,

$$\widetilde{\mathfrak{pDM}} := \left\{ \rho \in \widetilde{\mathfrak{DM}} \mid \exists \Psi \in \mathfrak{F}, \|\Psi\| = 1 : \rho = |\Psi\rangle\langle\Psi| \right\}, \quad (\text{I.24})$$

and

$$\mathfrak{pDM} := \mathfrak{DM} \cap \widetilde{\mathfrak{pDM}}. \quad (\text{I.25})$$

Another class of states that play an important role in our work is the set of *centered* density matrices,

$$\mathfrak{cDM} := \left\{ \rho \in \mathfrak{DM} \mid \forall f \in \mathcal{Z} : \text{Tr}_{\mathfrak{F}}[\rho a^*(f)] = 0 \right\}. \quad (\text{I.26})$$

I.3 Bogolubov-Hartree-Fock Energy

The determination of $E_{\text{gs}}(g, \vec{p})$ and the corresponding ground state $\rho_{\text{gs}}(g, \vec{p}) \in \mathfrak{DM}$ (provided the infimum is attained) is a difficult task. In this paper we rather study approximations to $E_{\text{gs}}(g, \vec{p})$ and $\rho_{\text{gs}}(g, \vec{p})$ that we borrow from the quantum mechanics of atoms and molecules, namely, the Bogolubov-Hartree-Fock (BHF) approximation. We define the BHF energy as

$$E_{BHF}(g, \vec{p}, \sigma, \Lambda) = \inf \left\{ \text{Tr}_{\mathfrak{F}} [\rho H_{g, \vec{p}}(\sigma, \Lambda)] \mid \rho \in \mathfrak{QF} \right\}, \quad (\text{I.27})$$

with corresponding BHF ground state(s) $\rho_{BHF}(g, \vec{p}, \sigma, \Lambda) \in \mathfrak{QF}$, determined by

$$\text{Tr}_{\mathfrak{F}} [\rho_{BHF}(g, \vec{p}, \sigma, \Lambda) H_{g, \vec{p}}(\sigma, \Lambda)] = E_{BHF}(g, \vec{p}, \sigma, \Lambda), \quad (\text{I.28})$$

where

$$\mathfrak{QF} := \left\{ \rho \in \mathfrak{DM} \mid \rho \text{ is quasifree} \right\} \subseteq \mathfrak{DM} \quad (\text{I.29})$$

denotes the subset of quasifree density matrices. A density matrix $\rho \in \mathfrak{DM}$ is called *quasifree*, if there exist $f_{\rho} \in \mathcal{Z}$ and a positive, self-adjoint operator $h_{\rho} = h_{\rho}^* \geq 0$ on \mathcal{Z} such that

$$\langle W(\sqrt{2}f/i) \rangle_{\rho} := \text{Tr}_{\mathfrak{F}} [\rho W(\sqrt{2}f/i)] = \exp \left[2i \text{Im} \langle f_{\rho} | f \rangle - \langle f | (1 + h_{\rho}) f \rangle \right], \quad (\text{I.30})$$

for all $f \in \mathcal{Z}$, where

$$W(f) := \exp [i\Phi(f)] := \exp \left[\frac{i}{\sqrt{2}} (a^*(f) + a(f)) \right] \quad (\text{I.31})$$

denotes the Weyl operator corresponding to f and we write expectation values w.r.t. the density matrix ρ as $\langle \cdot \rangle_{\rho}$.

There are several important facts about quasifree density matrices, which do not hold true for general density matrices in \mathfrak{DM} . See, e.g., [3, 9, 5, 6]. The first such fact is that if $\rho \in \mathfrak{QF}$ is a quasifree density matrix then so is $W(g)^* \rho W(g) \in \mathfrak{QF}$, for any $g \in \mathcal{Z}$, as follows from the Weyl commutation relations

$$\forall f, g \in \mathcal{Z} : \quad W(f) W(g) = e^{-\frac{i}{2} \text{Im} \langle f | g \rangle} W(f + g). \quad (\text{I.32})$$

Choosing $g := -i\sqrt{2}f_{\rho}$, we find that $W(-i\sqrt{2}f_{\rho})^* \rho W(-i\sqrt{2}f_{\rho})$ is a centered quasifree density matrix, i.e.,

$$W(\sqrt{2}f_{\rho}/i)^* \rho W(\sqrt{2}f_{\rho}/i) \in \mathfrak{cQF} := \mathfrak{QF} \cap \mathfrak{cDM}. \quad (\text{I.33})$$

Next, we formulate a characterization of centered quasifree density matrices.

Lemma I.1. *Let $\rho \in \mathfrak{c}\mathfrak{DM}$ be a centered density matrix and denote $\langle A \rangle_\rho := \text{Tr}_{\mathfrak{F}}\{\rho A\}$. Then (i) \Leftrightarrow (ii) \Leftrightarrow (iii), where*

(i) $\rho \in \mathfrak{c}\mathfrak{QF}$ is centered and quasifree;

(ii) All odd correlation functions and all even truncated correlation functions of ρ vanish, i.e., for all $N \in \mathbb{N}$ and $\varphi_1, \dots, \varphi_{2N} \in \mathcal{Z}$, let either $b_n := a^*(\varphi_n)$ or $b_n := a(\varphi_n)$, for all $1 \leq n \leq 2N$. Then $\langle b_1 \cdots b_{2N-1} \rangle_\rho = 0$ and

$$\langle b_1 b_2 \cdots b_{2N} \rangle_\rho = \sum_{\pi \in \mathfrak{P}_{2N}} \langle b_{\pi(1)} b_{\pi(2)} \rangle_\rho \cdots \langle b_{\pi(2N-1)} b_{\pi(2N)} \rangle_\rho, \quad (\text{I.34})$$

where \mathfrak{P}_{2N} denotes the set of pairings, i.e., the set of all permutations $\pi \in \mathfrak{S}_{2N}$ of $2N$ elements such that $\pi(2n-1) < \pi(2n+1)$ and $\pi(2n-1) < \pi(2n)$, for all $1 \leq n \leq N-1$ and $1 \leq n \leq N$, respectively.

(iii) There exist two commuting quadratic, semibounded Hamiltonians

$$H = \sum_{i,j} \left\{ B_{i,j} a^*(\psi_i) a(\psi_j) + C_{i,j} a^*(\psi_i) a^*(\psi_j) + \overline{C_{i,j}} a(\psi_i) a(\psi_j) \right\} \quad (\text{I.35})$$

$$H' = \sum_{i,j} \left\{ B'_{i,j} a^*(\psi_i) a(\psi_j) + C'_{i,j} a^*(\psi_i) a^*(\psi_j) + \overline{C'_{i,j}} a(\psi_i) a(\psi_j) \right\} \quad (\text{I.36})$$

with $B = B^* \geq 0$, $C = C^T \in \mathcal{L}^2(\mathcal{Z})$, where $\{\psi_i\}_{i \in \mathbb{N}} \subseteq \mathcal{Z}$ is an orthonormal basis, such that $\exp(-H - \beta H')$ is trace class, for all $\beta < \infty$, and

$$\langle A \rangle_\rho = \lim_{\beta \rightarrow \infty} \left\{ \frac{\text{Tr}_{\mathfrak{F}}[A \exp(-H - \beta H')]}{\text{Tr}_{\mathfrak{F}}[\exp(-H - \beta H')]} \right\}, \quad (\text{I.37})$$

for all $A \in \mathcal{B}(\mathfrak{F})$.

Eq. (I.33) and the vanishing (ii) of the truncated correlation functions of a centered quasifree state imply that any quasifree state $\rho \in \mathfrak{QF}$ is completely determined by its one-point function $\langle a(\varphi) \rangle_\rho$ and its two-point function (one-particle reduced density matrix)

$$\Gamma[\gamma_\rho, \tilde{\alpha}_\rho] := \begin{pmatrix} \gamma_\rho & \tilde{\alpha}_\rho \\ \tilde{\alpha}_\rho^* & \mathbf{1} + \mathcal{J} \gamma_\rho \mathcal{J} \end{pmatrix} \in \mathcal{B}(\mathcal{Z} \oplus \mathcal{Z}), \quad (\text{I.38})$$

where the operators $\gamma_\rho, \tilde{\alpha}_\rho \in \mathcal{B}(\mathcal{Z})$ are defined as

$$\langle \varphi, \gamma_\rho \psi \rangle := \langle a^*(\psi) a(\varphi) \rangle_\rho \quad \text{and} \quad \langle \varphi, \tilde{\alpha}_\rho \psi \rangle := \langle a(\varphi) a(\mathcal{J}\psi) \rangle_\rho, \quad (\text{I.39})$$

and $\mathcal{J} : \mathcal{Z} \rightarrow \mathcal{Z}$ is a conjugation. The positivity of the density matrix ρ implies that $\Gamma[\gamma_\rho, \tilde{\alpha}_\rho] \geq 0$ and, in particular, $\gamma_\rho \geq 0$, too. Moreover, the additional finiteness of the particle number expectation value, which distinguishes \mathfrak{DM} from $\widetilde{\mathfrak{DM}}$, ensures that $\gamma_\rho \in \mathcal{L}^1(\mathcal{Z})$ is trace-class, namely,

$$\mathrm{Tr}_{\mathcal{Z}}[\gamma_\rho] = \langle N_f \rangle_\rho < \infty, \quad (\text{I.40})$$

and that $\tilde{\alpha}_\rho \in \mathcal{L}^2(\mathcal{Z})$ is Hilbert-Schmidt.

Similar to (I.24)-(I.25), we introduce pure quasifree density matrices,

$$\mathfrak{p}\mathfrak{QF} := \mathfrak{QF} \cap \widetilde{\mathfrak{pDM}}. \quad (\text{I.41})$$

A subset of $\mathfrak{p}\mathfrak{QF}$ of special interest is given by *coherent states*, i.e., pure quasifree states of the form $|W(-i\sqrt{2}f)\Omega\rangle\langle W(-i\sqrt{2}f)\Omega|$, which we collect in

$$\mathrm{coh} := \{|W(-i\sqrt{2}f)\Omega\rangle\langle W(-i\sqrt{2}f)\Omega| \mid f \in \mathcal{Z}\}. \quad (\text{I.42})$$

For these, $\gamma_\rho = \tilde{\alpha}_\rho = 0$.

Conversely, if $\gamma \in \mathcal{L}_+^1(\mathcal{Z})$ is a positive trace-class operator and $\tilde{\alpha} \in \mathcal{L}^2(\mathcal{Z})$ is a Hilbert-Schmidt operator such that $\Gamma[\gamma, \tilde{\alpha}] \geq 0$ is positive then there exists a unique centered quasifree density matrix $\rho \in \mathfrak{c}\mathfrak{QF}$ such that $\gamma = \gamma_\rho$ and $\alpha = \alpha_\rho$ are its one-particle reduced density matrices.

Summarizing these two relations, the set \mathfrak{QF} of quasifree density matrices is in one-to-one correspondence to the convex set

$$1-\mathrm{pdm} := \{(f, \gamma, \tilde{\alpha}) \in \mathcal{Z} \oplus \mathcal{L}_+^1(\mathcal{Z}) \oplus \mathcal{L}^2(\mathcal{Z}) \mid \Gamma[\gamma, \tilde{\alpha}] \geq 0\}. \quad (\text{I.43})$$

Note that coherent states correspond to elements of $1-\mathrm{pdm}$ of the form $(f, 0, 0)$.

Next, we observe in accordance with (I.43) that, if $\rho \in \mathfrak{QF}$ is quasifree then its energy expectation value $\langle H_{g,\vec{p}} \rangle_\rho$ is a functional of $(f_\rho, \gamma_\rho, \tilde{\alpha}_\rho)$, namely,

$$\langle H_{g,\vec{p}} \rangle_\rho = \mathcal{E}_{g,\vec{p}}(f_\rho, \gamma_\rho, \tilde{\alpha}_\rho), \quad (\text{I.44})$$

where

$$\begin{aligned} \mathcal{E}_{g,\vec{p}}(f, \gamma, \tilde{\alpha}) &= \frac{1}{2} \{ (\mathrm{Tr}[\gamma \vec{k}] + f^* \vec{k} f + 2\mathrm{Re}(f^* \vec{G}) - \vec{p})^2 \\ &\quad + \mathrm{Tr}[\gamma \vec{k} \cdot \gamma \vec{k}] + \mathrm{Tr}[\tilde{\alpha}^* \vec{k} \cdot \tilde{\alpha} \vec{k}] + \mathrm{Tr}[|\vec{k}|^2 \gamma] \\ &\quad + 2\mathrm{Re}((\vec{G} + \vec{k} f)^* \tilde{\alpha}(\vec{G} + \vec{k} f)) + \mathrm{Tr}[(2\gamma + \mathbf{1})(\vec{G} + \vec{k} f) \cdot (\vec{G} + \vec{k} f)^*] \} \\ &\quad + \mathrm{Tr}[\gamma |\vec{k}|] + f^* |\vec{k}| f. \end{aligned} \quad (\text{I.45})$$

Now we are in position to formulate our main results.

Theorem I.2. *Let $0 \leq \sigma < \Lambda < \infty$, $g \in \mathbb{R}$ and $\vec{p} \in \mathbb{R}^3$, $|\vec{p}| < 1$. Minimizing the energy over quasifree states is the same as minimizing the energy over pure quasifree states, i.e.,*

$$E_{BHF}(g, \vec{p}, \sigma, \Lambda) := \inf_{\rho \in \mathfrak{Q}_{\mathfrak{F}}} \text{Tr}[H_{g, \vec{p}} \rho] = \inf_{\rho \in \mathfrak{p}\mathfrak{Q}_{\mathfrak{F}}} \text{Tr}[H_{g, \vec{p}} \rho]. \quad (\text{I.46})$$

Theorem I.3 (Coherent States Case). *There exists a universal constant $C < \infty$ such that, for $0 \leq \sigma < \Lambda < \infty$, $g^2 \ln(\Lambda + 2) \leq C$ and $|\vec{p}| \leq 1/3$, there exists a unique $f_{g, \vec{p}}$ which minimizes $\mathcal{E}_{g, \vec{p}}(f) = \mathcal{E}_{g, \vec{p}}(f, 0, 0)$ in $L^2(S_{\sigma, \Lambda} \times \mathbb{Z}_2, (\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)dk)$.*

1. *The minimizer $f_{g, \vec{p}}$ solves the system of equations*

$$\begin{cases} f_{g, \vec{p}} &= \frac{\vec{u}_{g, \vec{p}} \cdot \vec{G}}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u}_{g, \vec{p}}}, \\ \vec{u}_{g, \vec{p}} &= \vec{p} - 2\text{Re}(f_{g, \vec{p}}^* \vec{G}) - f_{g, \vec{p}}^* \vec{k} f_{g, \vec{p}}, \end{cases}$$

with $|\vec{u}_{g, \vec{p}}| \leq |\vec{p}|$.

2. *For $0 \leq \sigma < \Lambda < \infty$,*

$$\inf_{f \in L^2(S_{\sigma, \Lambda} \times \mathbb{Z}_2)} \mathcal{E}_{g, \vec{p}}(f) = \inf_{f \in L^2(S_{\sigma, \Lambda} \times \mathbb{Z}_2, (\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)dk)} \mathcal{E}_{g, \vec{p}}(f) = \mathcal{E}_{g, \vec{p}}(f_{g, \vec{p}}),$$

and for $0 < \sigma < \Lambda < \infty$, $f_{g, \vec{p}} \in L^2(S_{\sigma, \Lambda} \times \mathbb{Z}_2)$.

3. *For fixed g , σ , Λ , and small values of $|\vec{p}|$, we have that*

$$\mathcal{E}_{g, \vec{p}}(f_{g, \vec{p}}) = \mathcal{E}_{g, \vec{p}}(0) - \vec{p} \cdot \vec{G}^* \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G} \cdot \vec{G}^*} \vec{G} \cdot \vec{p} + \mathcal{O}(|\vec{p}|^3).$$

We summarize in Theorem I.4 the information obtained in Sections VI to VIII.

Theorem I.4 (Quasifree States Case). *Let $0 < \sigma < \Lambda < \infty$. There exists $C > 0$ (possibly depending on σ and Λ) such that for all $|g|, |\vec{p}| < C$, there exists a unique $(f_{g, \vec{p}}, \gamma_{g, \vec{p}}, \tilde{\alpha}_{g, \vec{p}})$ which minimizes the energy $\mathcal{E}_{g, \vec{p}}(f, \gamma, \tilde{\alpha})$.*

1. *The dependence of $(f_{g, \vec{p}}, \gamma_{g, \vec{p}}, \tilde{\alpha}_{g, \vec{p}})$ on (g, \vec{p}) is smooth.*

2. *The functions $(f_{g, \vec{p}}, \gamma_{g, \vec{p}}, \tilde{\alpha}_{g, \vec{p}})$ satisfy*

$$\begin{aligned} f_{g, \vec{p}} &= \left(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|\right)^{-1} \vec{p} \cdot \vec{G} + \mathcal{O}(\|(g, \vec{p})\|^3), \\ \tilde{\alpha}_{g, \vec{p}} &= -\tilde{S}^{-1}(\vec{G} \cdot \vec{G}^*) + \mathcal{O}(\|(g, \vec{p})\|^3), \\ \gamma_{g, \vec{p}} + \gamma_{g, \vec{p}}^2 &= \tilde{\alpha}_{g, \vec{p}} \tilde{\alpha}_{g, \vec{p}}^*, \end{aligned}$$

where \tilde{S} acts on the kernel $K_A(k, k')$ of a Hilbert-Schmidt operator A as the multiplication by $\vec{k} \cdot \vec{k}' + \frac{1}{2}|\vec{k}|^2 + |\vec{k}| + \frac{1}{2}|\vec{k}'|^2 + |\vec{k}'|$.

3. For fixed σ, Λ , and small values of $|g|$ and $|\vec{p}|$, we have that

$$E_{BHF}(g, \vec{p}, \sigma, \Lambda) = \mathcal{E}_{g, \vec{p}}(0, 0, 0) - g^2 |\vec{p}|^2 C_{2,2}(\sigma, \Lambda) - g^4 C_{4,0}(\sigma, \Lambda) + \mathcal{O}(\|(g, \vec{p})\|^5),$$

as $(g, \vec{p}) \rightarrow 0$, with $C_{2,2}(\sigma, \Lambda) = (2\pi^2 - \frac{8}{3}\pi) \ln(\frac{\Lambda+2}{\sigma+2})$ and $C_{4,0}(\sigma, \Lambda) > 0$.

4. The minimizer $(f_{g, \vec{p}}, \gamma_{g, \vec{p}}, \tilde{\alpha}_{g, \vec{p}})$ satisfies (we drop the g, \vec{p} indexes to simplify the notation)

$$\begin{aligned} M(\gamma, \vec{u})f &= -(\vec{k}(\gamma + \frac{1}{2}\mathbf{1}) - \vec{u}) \cdot \vec{G} - \vec{k} \cdot \tilde{\alpha}(\vec{G} + \vec{k}f), \\ \mathcal{A}(\lambda)\tilde{\alpha} &= -(\vec{G} + \vec{k}f) \cdot (\vec{G} + \vec{k}f)^*, \\ \gamma + \gamma^2 &= \tilde{\alpha} \tilde{\alpha}^*, \\ \lambda &:= \int_0^\infty e^{-t(\frac{1}{2}+\gamma)} (M(\gamma, \vec{u}) + (\vec{G} + \vec{k}f) \cdot (\vec{G} + \vec{k}f)^*) e^{-t(\frac{1}{2}+\gamma)} dt, \\ \vec{u} &:= \vec{p} - \text{Tr}[\gamma \vec{k}] - f^* \vec{k} f - 2\text{Re}(f^* \vec{G}), \end{aligned}$$

with

$$\begin{aligned} M(\gamma, \vec{u}) &:= \frac{1}{2} |\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u} + \vec{k} \cdot \gamma \vec{k}, \\ \mathcal{A}(\lambda)\tilde{\alpha} &:= \vec{k} \tilde{\alpha} \cdot \vec{k} + \lambda \tilde{\alpha} + \tilde{\alpha} \lambda. \end{aligned}$$

Remark I.5. In the coherent states case the formula

$$\mathcal{E}_{g, \vec{p}}(f_{g, \vec{p}}) = \mathcal{E}_{g, \vec{p}}(0) - g^2 |\vec{p}|^2 C_{2,2}(\sigma, \Lambda) + \mathcal{O}(\|(g, \vec{p})\|^5),$$

holds and can easily be compared to the quasifree state case.

Remark I.6. Although Theorem I.4 is formulated in terms of the one-particle reduced density matrix Γ_ρ and its constituents γ_ρ and $\tilde{\alpha}_\rho$, it turns out to be more convenient to parametrize the pureness constraint $\gamma_\rho + \gamma_\rho^2 = \tilde{\alpha}_\rho \tilde{\alpha}_\rho^*$ in terms of an anti-linear Hilbert-Schmidt operator \hat{r} which is chosen such that $\gamma_\rho = \frac{1}{2}(\cosh(2\hat{r}) - \mathbf{1})$, $\tilde{\alpha}_\rho = \frac{1}{2} \sinh(2\hat{r}) \mathcal{J}$, where $\mathcal{J} : f \in L^2(S_{\sigma, \Lambda} \times \mathbb{Z}_2) \mapsto \bar{f} \in L^2(S_{\sigma, \Lambda} \times \mathbb{Z}_2)$. This is explained in detail in Section III.

Outline of the article We introduce our notation to describe the second quantization framework in Section II. Section III introduces two parametrizations of pure quasifree states and contains the proof of Theorem I.2. The energy functional for a fixed value of the momentum \vec{p} of the dressed electron is computed in Section IV, along with some positivity properties of the different parts of the

energy. From Section V on we tacitly assume that the coupling constant $|g| > 0$ is small. The energy is then minimized in the particular case of coherent states in Section V, providing a first upper bound to the energy of the ground state and a proof of Theorem I.3. The existence and uniqueness of a minimizer among the class of pure quasifree state is then proven in Section VI provided $|\vec{p}|$ is small enough. The first terms of a perturbative expansion for small g and \vec{p} of the energy at the minimizer is computed in Section VII. Finally the Lagrange equations associated with the problem of minimization in the generalized one particle density matrix variables are presented in Section VIII.

II Second Quantization

In this section \mathcal{Z} denotes a \mathbb{C} -Hilbert space with a scalar product \mathbb{C} -linear in the right variable and \mathbb{C} -antilinear in the left variable.

Let $\mathcal{B}(X; Y)$ be the space of bounded operators between two Banach spaces X and Y , and $\mathcal{L}^1(\mathcal{Z})$ the space of trace class operators on \mathcal{Z} . Given two \mathbb{C} -Hilbert spaces $(\mathcal{Z}_j, \langle \cdot, \cdot \rangle_j)$, $j = 1, 2$ and a bounded linear operator $A : \mathcal{Z}_1 \rightarrow \mathcal{Z}_2$, set $A^* : \mathcal{Z}_2 \rightarrow \mathcal{Z}_1$ to be the operator such that

$$\forall z_1 \in \mathcal{Z}_1, z_2 \in \mathcal{Z}_2, \quad \langle z_2, Az_1 \rangle_2 = \overline{\langle z_1, A^*z_2 \rangle_1},$$

and $\operatorname{Re} A := \frac{1}{2}(A \oplus A^*)$, $\operatorname{Im} A := \frac{1}{2i}(A \oplus (-A^*)) \in \mathcal{B}(\mathcal{Z}_1, \mathcal{Z}_2) \oplus \mathcal{B}(\mathcal{Z}_2, \mathcal{Z}_1)$.

Example II.1. For $z, z' \in \mathcal{Z}$,

$$\langle z, z' \rangle = z^* z'.$$

The adjoint of a bounded operator A on \mathcal{Z} is A^* .

The symmetrization operator \mathcal{S}_n on $\mathcal{Z}^{\otimes n}$ is the orthogonal projection defined by

$$\mathcal{S}_n(z_1 \otimes \cdots \otimes z_n) = \frac{1}{n!} \sum_{\pi \in \mathfrak{S}_n} z_{\pi_1} \otimes \cdots \otimes z_{\pi_n}$$

and extension by linearity and continuity. The symmetric tensor product for vectors is $z_1 \vee z_2 = \mathcal{S}_{n_1+n_2}(z_1 \otimes z_2)$ and more generally for operators is $A_1 \vee A_2 = \mathcal{S}_{q_1+q_2} \circ (A_1 \otimes A_2) \circ \mathcal{S}_{p_1+p_2}$ for $A_j \in \mathcal{B}(\mathcal{Z}^{\otimes p_j}; \mathcal{Z}^{\otimes q_j})$. We set

$$\mathcal{Z}^{\vee n} := \mathcal{S}_n \mathcal{Z}^{\otimes n}, \quad \mathcal{B}^{p,q} := \mathcal{B}(\mathcal{Z}^{\otimes p}; \mathcal{Z}^{\otimes q}).$$

Definition II.2. The symmetric Fock space on a Hilbert space \mathcal{Z} is defined to be

$$\mathfrak{F}_+(\mathcal{Z}) := \bigoplus_{n=0}^{\infty} \mathcal{Z}^{\vee n},$$

where $\mathcal{Z}^{\vee 0} := \mathbb{C}\Omega$, Ω being the normalized vacuum vector.

For a linear operator C on \mathcal{Z} such that $\|C\|_{\mathcal{B}(\mathcal{Z})} \leq 1$, let $\Gamma(C)$ defined on each $\mathcal{Z}^{\vee n}$ by $C^{\vee n}$ and extended by continuity to the symmetric Fock space on \mathcal{Z} .

For an operator X on \mathcal{Z} , the second quantization $d\Gamma(X)$ of X is defined on each $\mathcal{Z}^{\vee n}$ by

$$d\Gamma(X) \Big|_{\mathcal{Z}^{\vee n}} = n \mathbf{1}_{\mathcal{Z}}^{\vee n-1} \vee X$$

and extended by linearity to $\bigoplus_{n \geq 0}^{alg} \mathcal{Z}^{\vee n}$. The number operator is $N_f = d\Gamma(\mathbf{1}_{\mathcal{Z}})$. For a vector f in \mathcal{Z} , the creation and annihilation operators in f are the linear operators such that $a(f)\Omega = 0$, $a^*(f)\Omega = f$, and

$$a(f)g^{\vee n} = \sqrt{n}(f^*g) g^{\vee n-1}, \quad \text{and} \quad a^*(f)g^{\vee n} = \sqrt{n+1}f \vee g^{\vee n}, \quad (\text{II.47})$$

for all $g \in \mathcal{Z}$. By the polarization identity

$$\forall g_1, \dots, g_n, \quad g_1 \vee \dots \vee g_n = \frac{1}{2^n n!} \sum_{\varepsilon_i = \pm 1} \varepsilon_1 \dots \varepsilon_n \left(\sum_{j=1}^n \varepsilon_j g_j \right)^{\otimes n}$$

Eq. (II.47) extends to $\mathcal{Z}^{\vee n}$ and hence also to $\bigoplus_{n \geq 0}^{alg} \mathcal{Z}^{\vee n}$. They satisfy the canonical commutation relations $[a(f), a^*(g)] = f^*g$, $[a(f), a(g)] = [a^*(f), a^*(g)] = 0$.

The self-adjoint field operator associated to f is $\Phi(f) = \frac{1}{\sqrt{2}}(a^*(f) + a(f))$. For more details on the second quantization see the book of Berezin [4].

A dot “ \cdot ” denotes an operation analogous to the scalar product in \mathbb{R}^3 . For every two objects $\vec{a} = (a_1, a_2, a_3)$ and $\vec{b} = (b_1, b_2, b_3)$ with three components such that the products $a_j b_j$ are well defined

$$\vec{a} \cdot \vec{b} := \sum_{j=1}^3 a_j b_j.$$

Example II.3. With $\vec{p} \in \mathbb{R}^3$, $\vec{G} \in \mathcal{Z}^3$, $\vec{k} \in (\mathcal{B}^{1,1})^3$

$$\begin{aligned} \vec{p}^{\cdot 2} &= \sum_{j=1}^3 p_j^2 \in \mathbb{R}, & \vec{k} \cdot \vec{p} &= \sum_{j=1}^3 p_j k_j \in \mathcal{B}^{1,1}, & \vec{p} \cdot \vec{G} &= \sum_{j=1}^3 p_j G_j \in \mathcal{Z}, \\ \vec{k}^{\cdot 2} &= \sum_{j=1}^3 k_j^2 \in \mathcal{B}^{1,1}, & \vec{k} \cdot \vec{G} &= \sum_{j=1}^3 k_j G_j \in \mathcal{Z}, & \vec{G}^* \cdot \vec{k} &= \sum_{j=1}^3 G_j^* k_j \in \mathcal{Z}^*, \\ \vec{G} \cdot \vec{G}^* &= \sum_{j=1}^3 G_j G_j^* \in \mathcal{B}^{1,1}, & \vec{G}^* \cdot \vec{G} &= \sum_{j=1}^3 G_j^* G_j \in \mathbb{C}, \end{aligned}$$

where for an object with three components $\vec{a} = (a_1, a_2, a_3)$ such that a_j^* is well-defined, $\vec{a}^* := (a_1^*, a_2^*, a_3^*)$. We sometimes use the notation $\vec{p}^{\cdot 2} = |\vec{p}|^2$, or $\vec{k}^{\cdot 2} = |\vec{k}|^2$.

And with another product, such as the symmetric tensor product \vee ,

$$\vec{k}^{\cdot \vee 2} = \sum_{j=1}^3 k_j^{\vee 2} \in \mathcal{B}^{2,2}, \quad \vec{k}^{\cdot \vee} \vec{G} = \sum_{j=1}^3 k_j \vee G_j \in \mathcal{B}^{2,3}.$$

Recall that the Weyl operators are the unitary operators $W(f) = \exp(i\Phi(f))$ satisfying the relations

$$\forall z_1, z_2 \in \mathcal{Z} : \quad W(z_1)W(z_2) = e^{-\frac{i}{2}\text{Im}(z_1^* z_2)} W(z_1 + z_2), \quad (\text{II.48})$$

$$\forall z \in \mathcal{Z} : \quad W(-i\sqrt{2}z)\Omega = e^{-\frac{|z|^2}{2}} \sum_{n=0}^{\infty} \frac{z^{\vee n}}{\sqrt{n!}}. \quad (\text{II.49})$$

Definition II.4. The *coherent vectors* are the vectors of the form

$$E_z = W(-i\sqrt{2}z)\Omega$$

for some $z \in \mathcal{Z}$ and the *coherent states* are the states of the form

$$E_z E_z^*.$$

Definition II.5. A *symplectomorphism* T for the symplectic form $\text{Im}\langle \cdot, \cdot \rangle$ on a \mathbb{C} -Hilbert space \mathcal{Z} is a continuous \mathbb{R} -linear automorphism on \mathcal{Z} which preserves this symplectic form, i.e.,

$$\forall z_1, z_2 \in \mathcal{Z} : \quad \text{Im}\langle Tz_1, Tz_2 \rangle = \text{Im}\langle z_1, z_2 \rangle.$$

A symplectomorphism T is *implementable* if there is a unitary operator \mathbb{U}_T on $\mathfrak{F}_+(\mathcal{Z})$ such that

$$\forall z \in \mathcal{Z}, \quad \mathbb{U}_T W(z) \mathbb{U}_T^* = W(Tz).$$

In this case \mathbb{U}_T is a *Bogolubov transformation* corresponding to T .

We recall a well-known parametrization, in the spirit of the polar decomposition, of implementable symplectomorphisms.

Proposition II.6. *The set of implementable symplectomorphisms is the set of operators*

$$T = u \exp[\hat{r}] = u \sum_{n=0}^{\infty} \frac{1}{n!} \hat{r}^n,$$

where u is an isometry and \hat{r} is an antilinear operator, self-adjoint in the sense that $\forall z, z' \in \mathcal{Z}$, $\langle z, \hat{r}z' \rangle = \langle z', \hat{r}z \rangle$, and Hilbert-Schmidt in the sense that the positive operator \hat{r}^2 is trace-class. Equivalently, there exist a Hilbert basis $(\varphi_j)_{j \in \mathbb{N}}$ of \mathcal{Z} and $(\hat{r}_{i,j})_{i,j} \in \ell^2(\mathbb{N}^2; \mathbb{C})$ such that

$$\hat{r} = \sum_{i,j=1}^{\infty} \hat{r}_{i,j} \langle \cdot, \varphi_j \rangle \varphi_i \quad \text{and} \quad \forall i, j \in \mathbb{N}^2 : \quad \hat{r}_{i,j} = \hat{r}_{j,i}.$$

Proof. On the one hand, every operator of the form $T = u \exp[\hat{r}]$ with u a unitary operator and \hat{r} a self-adjoint antilinear operator is a symplectomorphism. Since a unitary operator is a symplectomorphism, and the set of symplectomorphisms is a group for the composition, it is enough to prove that $\exp[\hat{r}]$ is a symplectomorphism. It is indeed the case since, for all z, z' in \mathcal{Z} ,

$$\begin{aligned} \operatorname{Im} \langle e^{\hat{r}} z, e^{\hat{r}} z' \rangle &= \operatorname{Im} \langle e^{\hat{r}} z, \cosh(\hat{r}) z' \rangle + \operatorname{Im} \langle e^{\hat{r}} z, \sinh(\hat{r}) z' \rangle \\ &= \operatorname{Im} \langle \cosh(\hat{r}) e^{\hat{r}} z, z' \rangle + \operatorname{Im} \langle z', \sinh(\hat{r}) e^{\hat{r}} z \rangle \\ &= \operatorname{Im} \langle \cosh(\hat{r}) e^{\hat{r}} z, z' \rangle - \operatorname{Im} \langle \sinh(\hat{r}) e^{\hat{r}} z, z' \rangle \\ &= \operatorname{Im} \langle e^{-\hat{r}} e^{\hat{r}} z, z' \rangle. \end{aligned}$$

The implementability condition is then satisfied if we suppose \hat{r} to be Hilbert-Schmidt.

On the other hand, to get exactly this formulation we give the step to go from the result given in Appendix A in [7] to the decomposition in Proposition II.6. In [7] an implementable symplectomorphism is decomposed as

$$T = u e^{c\tilde{r}}, \quad (\text{II.50})$$

where u is a unitary operator, c is a conjugation and \tilde{r} is a Hilbert-Schmidt, self-adjoint, non-negative operator commuting with c . It is then enough to set $\hat{r} = c\tilde{r}$ to get the expected decomposition. To check the self-adjointness of \hat{r} , observe that, for all z, z' in \mathcal{Z} ,

$$\langle z', \hat{r}z \rangle = \langle z', \tilde{r}cz \rangle = \langle \tilde{r}z', cz \rangle = \langle z, c\tilde{r}z' \rangle = \langle z, \hat{r}z' \rangle.$$

For the convenience of the reader we recall the main steps to obtain the decomposition in Eq. (II.50). First decompose T in its \mathbb{C} -linear and antilinear parts, $T = L + A$, then write the polar decomposition $L = u|L|$. It is then enough to prove that $|L| + u^*A$ is of the form $e^{c\tilde{r}}$. From certain properties of symplectomorphisms (also recalled in [7]) it follows that the antilinear operator u^*A is selfadjoint and $|L|^2 + \mathbf{1}_{\mathcal{Z}} = (u^*A)^2$. A decomposition of the positive trace class operator $(u^*A)^2 = \sum_j \lambda_j^2 e_j e_j^*$ with e_j an orthonormal basis of \mathcal{Z} yields

$|L| = \sum_j (1 + \lambda_j^2)^{1/2} e_j e_j^*$. Using that $\lambda_j \rightarrow 0$ one can study the operator $|L|$ and $u^* A$ on the finite dimensional subspaces $\ker(|L| - \mu \mathbf{1}_{\mathcal{Z}})$ which are invariant under $u^* A$. It is then enough to prove that for a \mathbb{C} -antilinear self-adjoint operator f such that $f f^* = \lambda^2$ on a finite dimensional space, there is an orthonormal basis $\{\varphi_k\}_k$ such that $f(\varphi_k) = \lambda \varphi_k$. The conjugation is then defined such that $c(\sum \beta_k \varphi_k) = \sum \bar{\beta}_k \varphi_k$ and $\tilde{r} = \sinh^{-1}(\lambda_j) \mathbf{1}$ on that subspace. \square

III Pure Quasifree States

III.1 From Quasifree States to Pure Quasifree States

Let \mathcal{Z} be the \mathbb{C} -Hilbert space $L^2(S_{\sigma, \Lambda} \times \mathbb{Z}_2)$. We make use of the following characterization of quasifree density matrices.

Lemma III.1. *The set of quasifree density matrices and pure quasifree density matrices, respectively, of finite photon number expectation value can be characterized by*

$$\begin{aligned} \Omega\mathfrak{F} = \mathfrak{DM} \bigcap \Big\{ & W(-i\sqrt{2}f) \mathbb{U}^* \frac{\Gamma(C)}{\text{Tr}[\Gamma(C)]} \mathbb{U} W(-i\sqrt{2}f)^* \\ & \Big| \begin{aligned} & f \in \mathcal{Z}, \mathbb{U} \text{ a Bogolubov transformation,} \\ & C \in \mathcal{L}^1(\mathcal{Z}), C \geq 0, \|C\|_{\mathcal{B}(\mathcal{Z})} < 1 \end{aligned} \Big\} \end{aligned}$$

$$\begin{aligned} \text{p}\Omega\mathfrak{F} = \mathfrak{DM} \bigcap \Big\{ & W(-i\sqrt{2}f) \mathbb{U}^* \Omega \Omega^* \mathbb{U} W(-i\sqrt{2}f)^* \\ & \Big| f \in \mathcal{Z}, \mathbb{U} \text{ a Bogolubov transformation} \Big\} \end{aligned}$$

Proof. We only sketch the argument, details can be found in [4, 9]. It is not difficult to see that any density matrix of the form $W(-i\sqrt{2}f) \mathbb{U}^* \frac{\Gamma(C)}{\text{Tr}[\Gamma(C)]} \mathbb{U} W(-i\sqrt{2}f)^*$ is indeed quasifree. Conversely, if $\rho \in \Omega\mathfrak{F}$ is a quasifree density matrix then it is fully characterized by its one-point function $f_\rho \in \mathcal{Z}$ and two-point functions $(\gamma_\rho, \tilde{\alpha}_\rho)$. Moreover, $W(-i\sqrt{2}f_\rho)^* \rho W(-i\sqrt{2}f_\rho) \in \mathfrak{c}\Omega\mathfrak{F}$ is a centered quasifree density matrix with the same one-particle density matrix, that is, the density matrix $W(-i\sqrt{2}f_\rho)^* \rho W(-i\sqrt{2}f_\rho)$ corresponds to $(0, \gamma_\rho - f_\rho f_\rho^*, \tilde{\alpha}_\rho - f_\rho \tilde{f}_\rho^*)$. Obviously, $\gamma_\rho - f_\rho f_\rho^*$ is again trace-class and $\tilde{\alpha}_\rho - f_\rho \tilde{f}_\rho^*$ is Hilbert-Schmidt. Now, we use that there exists a Bogolubov transformation \mathbb{U} which eliminates $\tilde{\alpha}_\rho$, i.e., $\mathbb{U}^* W(\sqrt{2}f_\rho/i)^* \rho W(\sqrt{2}f_\rho/i) \mathbb{U}$ corresponds to $(0, \tilde{\gamma}_\rho, 0)$. While this is the only nontrivial step of the proof, we note that if \mathbb{U} is characterized by u and v as in Lemma III.2 then there is an involved, but explicit formula that determines u and

v. Again $\tilde{\gamma}_\rho$ is trace-class because the photon number operator N_f transforms under \mathbb{U}^* to itself plus lower order corrections, $\mathbb{U}^* N_f \mathbb{U} = N_f + \mathcal{O}(N_f^{1/2} + 1)$. Finally, it is easy to see that $(0, \tilde{\gamma}_\rho, 0)$ corresponds to the quasifree density matrix $\Gamma(C_\rho)/\text{Tr}[\Gamma(C_\rho)]$ with $C_\rho := \tilde{\gamma}_\rho(1 + \tilde{\gamma}_\rho)^{-1}$. Following these steps we finally obtain

$$\rho = W(f_\rho) \mathbb{U} \frac{\Gamma(C_\rho)}{\text{Tr}[\Gamma(C_\rho)]} \mathbb{U}^* W(f_\rho)^*,$$

as asserted. The additional characterization of pure quasifree density matrices is obvious. \square

Lemma III.2. *Let $\mathbb{U} \in \mathcal{B}(\mathfrak{F})$ be a unitary operator. The following statements are equivalent:*

$$\mathbb{U} \in \mathcal{B}(\mathfrak{F}) \text{ is a Bogolubov transformation;} \quad (\text{III.51})$$

$$\Leftrightarrow \exists T \text{ implementable symplectomorphism,} \quad (\text{III.52})$$

$$\mathbb{U} = \tilde{U}_T, \quad \tilde{U}_T W(f) \tilde{U}_T^* = W(Tf).$$

$$\Leftrightarrow \exists u \in \mathcal{B}(\mathcal{Z}), v \in \mathcal{L}^2(\mathcal{Z}) \forall f \in \mathcal{Z} : \quad (\text{III.53})$$

$$\mathbb{U} a^*(f) \mathbb{U}^* = a^*(uf) + a(\mathcal{J}v \mathcal{J}f);$$

$$\Leftrightarrow \mathbb{U} = \exp(iH), \text{ where } H = H^* \text{ is a semibounded operator,} \quad (\text{III.54})$$

quadratic in a^ and a and without linear term.*

Proof. Again, we only sketch the argument. First note that (III.51) \Leftrightarrow (III.52) is the definition of a Bogolubov transformation. Secondly, $\tilde{U}_T W(f) \tilde{U}_T^* = W(Tf)$ is equivalent to $\tilde{U}_T \Phi(f) \tilde{U}_T^* = \Phi(Tf)$. Hence, using that $a^*(f) = \frac{1}{\sqrt{2}}[\Phi(f) - i\Phi(if)]$ and $a(f) = \frac{1}{\sqrt{2}}[\Phi(f) + i\Phi(if)]$ we obtain the equivalence (III.52) \Leftrightarrow (III.53). Thirdly, setting $U_\lambda = \exp(i\lambda H)$ and $a_\lambda^*(f) := U_\lambda a^*(f) U_\lambda^*$, we observe that $\partial_\lambda a_\lambda^*(f) = i[H, a_\lambda^*(f)]$. Furthermore, $[H, a_\lambda^*(f)]$ is linear in a^* and a if, and only if, H is quadratic in a^* and a . Solving this linear differential equation, we finally obtain (III.53) \Leftrightarrow (III.54). \square

Lemma III.3. *For all Bogolubov transformation \mathbb{U} and $g \in \mathcal{Z}$:*

$$W(g) \mathbb{U} \mathfrak{Q} \mathfrak{F} \mathbb{U}^* W(g)^* = \mathfrak{Q} \mathfrak{F}, \quad (\text{III.55})$$

$$\mathbb{U} \mathfrak{c} \mathfrak{Q} \mathfrak{F} \mathbb{U}^* = \mathfrak{c} \mathfrak{Q} \mathfrak{F}. \quad (\text{III.56})$$

Remark III.4. A pure quasifree state is a particular case of quasifree state with $C = 0$, that is $\Gamma(C) = \Omega \Omega^*$.

We come to the main result of this section.

Theorem III.5. *Let $0 \leq \sigma < \Lambda < \infty$, $g \in \mathbb{R}$ and $\vec{p} \in \mathbb{R}^3$, $|\vec{p}| < 1$. Minimizing the energy over quasifree states is the same as minimizing the energy over pure quasifree states, i.e.,*

$$E_{BHF}(g, \vec{p}, \sigma, \Lambda) := \inf_{\rho \in \mathfrak{Q}\mathfrak{F}} \text{Tr}[H_{g, \vec{p}} \rho] = \inf_{\rho \in \mathfrak{p}\mathfrak{Q}\mathfrak{F}} \text{Tr}[H_{g, \vec{p}} \rho].$$

For the proof of Theorem III.5 we derive a couple of preparatory lemmata.

Proposition III.6. *Let C a non-negative operator on \mathcal{Z} , then*

$$\left\{ \text{Tr}[\Gamma(C)] < \infty \right\} \Leftrightarrow \left\{ C \in \mathcal{L}^1(\mathcal{Z}) \text{ and } \|C\|_{\mathcal{B}(\mathcal{Z})} < 1 \right\}.$$

In this case $\text{Tr}[\Gamma(C)] = \det(1 - C)^{-1}$. (We refrain from defining the determinant.) For the direction \Leftarrow the non-negativity assumption is not necessary.

Proof. Let us decompose $\mathcal{Z} = \bigoplus_{j \geq 0} \mathbb{C}e_j$ where $C = \sum c_j e_j e_j^*$ with $(e_j)_{j \geq 0}$ an orthonormal basis of \mathcal{Z} . Then $\mathfrak{F}_+(\mathcal{Z}) = \bigotimes_{j \geq 0} \mathfrak{F}_+(\mathbb{C}e_j)$ and

$$\text{Tr}[\Gamma(C)] = \text{Tr}\left[\bigotimes_{j \geq 0} \Gamma(c_j)\right] = \prod_{j \geq 0} \text{Tr}[\Gamma(c_j)] = \prod_{j \geq 0} \frac{1}{1 - c_j}$$

and the infinite product converges exactly when $C \in \mathcal{L}^1(\mathcal{Z})$ and $\|C\|_{\mathcal{B}(\mathcal{Z})} < 1$. \square

Lemma III.7. *Suppose \mathcal{Z}_d is of dimension $d < \infty$. Then, for any non-negative operator $C_d \neq 0$ such that $C_d \in \mathcal{L}^1(\mathcal{Z}_d)$ and $\|C_d\|_{\mathcal{B}(\mathcal{Z}_d)} < 1$, there exist a non-negative measure μ_d (depending on C) of mass one on \mathcal{Z}_d and a family $\{\rho_d(z_d)\}_{z_d \in \mathcal{Z}_d}$ of pure quasifree states such that*

$$\frac{\Gamma(C)}{\text{Tr}[\Gamma(C)]} = \int_{\mathcal{Z}_d} \rho_d(z_d) d\mu_d(z_d).$$

Proof. In finite dimension d we can use a resolution of the identity with coherent states (see, e.g., [4])

$$\mathbf{1}_{\Gamma(\mathcal{Z}_d)} = \int_{\mathcal{Z}_d} E_{z_d} E_{z_d}^* \frac{dz_d}{\pi^d}$$

where \mathcal{Z}_d is identified with \mathbb{C}^d and $dz_d = dx_d dy_d$, $z_d = x_d + iy_d$. Using Equation (II.49) we get

$$\begin{aligned} \Gamma(C) &= \int_{\mathcal{Z}_d} \Gamma(C^{1/2}) E_{z_d} E_{z_d}^* \Gamma(C^{1/2}) \frac{dz_d}{\pi^d} \\ &= \int_{\mathcal{Z}_d} E_{C^{1/2} z_d} E_{C^{1/2} z_d}^* \frac{\exp(|C^{1/2} z_d|^2 - |z_d|^2) dz_d}{\pi^d}. \end{aligned}$$

The measure $d\mu_d(z_d) = \pi^{-d} \exp(|C^{1/2}z_d|^2 - |z_d|^2) dz_d / \text{Tr}[\Gamma(C)]$ has mass one. Indeed

$$\begin{aligned} \int_{\mathcal{Z}_d} \exp(-z_d^*(\mathbf{1}_{\mathcal{Z}_d} - C)z_d) \frac{dz_d}{\pi^d} &= \prod_{j=1}^d \int_{\mathbb{R}^2} \exp(-(1 - c_j)(x^2 + y^2)) \frac{dx dy}{\pi} \\ &= \prod_{j=1}^d \frac{1}{1 - c_j} = \text{Tr}[\Gamma(C)] \end{aligned}$$

where $C = \sum_{j=1}^d c_j e_j e_j^*$ with $(e_j)_{j=1}^d$ an orthonormal basis of \mathcal{Z}_d . \square

Proof of Theorem III.5. The inclusion $\mathfrak{p}\mathfrak{Q}\mathfrak{F} \subset \mathfrak{Q}\mathfrak{F}$ implies that

$$\inf_{\rho \in \mathfrak{Q}\mathfrak{F}} \text{Tr}[H_{g,\vec{p}} \rho] \leq \inf_{\rho \in \mathfrak{p}\mathfrak{Q}\mathfrak{F}} \text{Tr}[H_{g,\vec{p}} \rho],$$

and it is hence enough to prove for any quasifree state

$$\rho_{qf} = W(-i\sqrt{2}f) \mathbb{U}_T^* \frac{\Gamma(C)}{\text{Tr}[\Gamma(C)]} \mathbb{U}_T W(-i\sqrt{2}f)^*,$$

that the inequality

$$\text{Tr}[H_{g,\vec{p}} \rho_{qf}] \geq \inf_{\rho \in \mathfrak{p}\mathfrak{Q}\mathfrak{F}} \text{Tr}[H_{g,\vec{p}} \rho].$$

holds true. The operator C is decomposed as $C = \sum_{j \geq 0} c_j e_j e_j^*$ where (e_j) is an orthonormal basis of the Hilbert space \mathcal{Z} and $c_j \geq 0$. Let $C_d = \sum_{j \leq d} c_j e_j e_j^*$. Let

$$\rho_{qf,d} = W(-i\sqrt{2}f) \mathbb{U}_T^* \frac{\Gamma(C_d)}{\text{Tr}[\Gamma(C_d)]} \mathbb{U}_T W(-i\sqrt{2}f)^*,$$

then using Lemma III.7 with $\mathcal{Z}_d = \bigoplus_{j \leq d} \mathbb{C} e_j$, $\mathfrak{F}_+ \mathcal{Z} = \mathfrak{F}_+(\mathcal{Z}_d \oplus \mathcal{Z}_d^\perp) \cong \mathfrak{F}_+ \mathcal{Z}_d \otimes \mathfrak{F}_+ \mathcal{Z}_d^\perp$ and the extension of the operator $\Gamma(C_d)$ on $\mathfrak{F}_+ \mathcal{Z}_d$ to $\mathfrak{F}_+ \mathcal{Z}_d \otimes \mathfrak{F}_+ \mathcal{Z}_d^\perp$ by $\Gamma(C_d) \otimes (\Omega_{\mathcal{Z}_d^\perp} \Omega_{\mathcal{Z}_d^\perp}^*)$ (which we still denote by $\Gamma(C_d)$), we obtain

$$\rho_{qf,d} = \int_{\mathcal{Z}_d} \rho_d(z_d) d\mu_d(z_d),$$

where $\rho_d(z_d)$ are pure quasifree states and the μ_d are non-negative measures with mass one. Note that

$$\nu_d := \frac{\text{Tr}[\Gamma(C_d)]}{\text{Tr}[\Gamma(C)]} = \prod_{j > d} (1 - c_j) \nearrow 1,$$

as $d \rightarrow \infty$. Further note that $\rho_{qf} \geq \nu_d \rho_{qf,d}$, for any $d \in \mathbb{N}$, since $\Gamma(C) \geq \Gamma(C_d)$. Thus

$$\begin{aligned} \text{Tr}[H_{g,\vec{p}} \rho_{qf}] &\geq \text{Tr}[H_{g,\vec{p}} \nu_d \rho_{qf,d}] \\ &= \nu_d \int_{\mathcal{Z}_d} \text{Tr}[H_{g,\vec{p}} \rho_d(z_d)] d\mu_d(z_d) \\ &\geq \nu_d \inf_{z_d \in \mathcal{Z}_d} \text{Tr}[H_{g,\vec{p}} \rho_d(z_d)] \\ &\geq \nu_d \inf_{\rho \in \mathfrak{p}\Omega_{\mathfrak{F}}} \text{Tr}[H_{g,\vec{p}} \rho], \end{aligned}$$

for all $d \in \mathbb{N}$, and in the limit $d \rightarrow \infty$, we obtain

$$\text{Tr}[H_{g,\vec{p}} \rho_{qf}] \geq \lim_{d \rightarrow \infty} \{\nu_d\} \inf_{\rho \in \mathfrak{p}\Omega_{\mathfrak{F}}} \text{Tr}[H_{g,\vec{p}} \rho] = \inf_{\rho \in \mathfrak{p}\Omega_{\mathfrak{F}}} \text{Tr}[H_{g,\vec{p}} \rho]. \quad \square$$

III.2 Pure Quasifree States and their One-Particle Density Matrices

Let \mathcal{Z} be a \mathbb{C} -Hilbert space.

Definition III.8. Let $\rho \in \mathfrak{DM}$ be a density matrix on the bosonic Fock space $\mathfrak{F}_+(\mathcal{Z})$ over \mathcal{Z} . If $\text{Tr}[\rho N_f^{\frac{p+q}{2}}] < \infty$, we define $\rho^{p,q} \in \mathcal{B}^{p,q}(\mathcal{Z})$ through

$$\forall \varphi, \psi \in \mathcal{Z}, \quad \psi^{*\vee p} \rho^{p,q} \varphi^{\vee q} = \text{Tr}[a^*(\varphi)^q a(\psi)^p \rho].$$

We single out

$$f = \rho^{0,1} \in \mathcal{B}^{0,1} \cong \mathcal{Z},$$

i.e., $f_\rho \in \mathcal{Z}$ is the unique vector such that $\text{Tr}[a(\psi) \rho] = \psi^* f_\rho$, for all $\psi \in \mathcal{Z}$. Furthermore, with $\tilde{\rho} = W(\sqrt{2}f_\rho/i)^* \rho W(\sqrt{2}f_\rho/i)$, the matrix elements of the (generalized) one-particle density matrix are defined by

$$\gamma_\rho = \tilde{\rho}^{1,1} \in \mathcal{B}^{1,1} \quad \text{and} \quad \alpha_\rho = \tilde{\rho}^{0,2} \in \mathcal{B}^{0,2} \cong \mathcal{Z}^{\vee 2},$$

in other words

$$\begin{aligned} \forall \varphi, \psi \in \mathcal{Z} : \quad \langle \psi, \gamma_\rho \varphi \rangle &= \text{Tr}[\tilde{\rho} a^*(\varphi) a(\psi)], \\ \langle \psi \otimes \varphi, \alpha_\rho \rangle &= \text{Tr}[\tilde{\rho} a(\psi) a(\varphi)]. \end{aligned}$$

Note that f_ρ , γ_ρ , and α_ρ exist for any $\rho \in \mathfrak{DM}$ since $N_f \rho, \rho N_f \in \mathcal{L}^1(\mathfrak{F}_+)$.

Remark III.9. For a centered pure quasifree state $\tilde{\rho}$, $\tilde{\rho}^{p,q}$ vanishes when $p + q$ is odd.

Remark III.10. Another definition of the one-particle density matrix γ_ρ would be through the relation $\langle \psi, \gamma_\rho \varphi \rangle = \text{Tr}[a^*(\varphi)a(\psi)\rho]$. We prefer here a definition with a “centered” version $\tilde{\rho}$ of the state ρ , because this centered quasifree state $\tilde{\rho}$ then satisfies the usual Wick theorem. The same considerations hold for α_ρ .

Hence, any quasifree density matrix is characterized by $(f_\rho, \gamma_\rho, \alpha_\rho)$, since $\rho^{p,q}$ can be expressed in terms of $(f_\rho, \gamma_\rho, \alpha_\rho)$.

When $f_\rho = 0$, the definition of γ_ρ is consistent with the usual one, for $z_1, z_2 \in \mathcal{Z}$, $\langle z_1, \gamma_\rho z_2 \rangle = \text{Tr}[a^*(z_2)a(z_1)\rho]$. The definition of α_ρ is related with the definition of the operator $\hat{\alpha}_\rho$ (here denoted with a hat for clarity) used in the article of Bach, Lieb and Solovej [3], through the relation $\langle z_1 \otimes z_2, \alpha_\rho \rangle_{\mathcal{Z}^{\otimes 2}} = \langle z_1, \tilde{\alpha}_\rho c z_2 \rangle_{\mathcal{Z}}$ with c a conjugation on \mathcal{Z} .

Example III.11. A centered pure quasifree state satisfies the relation,

$$\tilde{\rho}^{2,2} = \gamma \otimes \gamma + \gamma \otimes \gamma \text{ Ex} + \alpha \alpha^* \in \mathcal{B}^{2,2}, \quad (\text{III.57})$$

where the exchange operator is the linear operator on $\mathcal{Z}^{\otimes 2}$ such that

$$\forall z_1, z_2 \in \mathcal{Z}, \quad \text{Ex}(z_1 \otimes z_2) = z_2 \otimes z_1$$

and where for any $b \in \mathcal{Z}^{\otimes 2}$, $\alpha \alpha^* b = \langle \alpha, b \rangle_{\mathcal{Z}^{\otimes 2}} \alpha$.

We now turn to another parametrization of quasifree states, by vectors in a real Hilbert space. This parametrization enables us to use convexity arguments.

Proposition III.12. *Let $T = ue^{\hat{r}}$ be an implementable symplectomorphism and ρ a quasifree state of the form $\rho = \mathbb{U}_T^* \Omega \Omega^* \mathbb{U}_T$. Then*

$$\gamma_\rho = \frac{1}{2}(\cosh(2\hat{r}) - 1), \quad (\text{III.58})$$

$$\forall z_1, z_2 \in \mathcal{Z} : \quad \langle z_1 \otimes z_2, \alpha_\rho \rangle_{\mathcal{Z}^{\otimes 2}} = \langle z_1, \frac{1}{2} \sinh(2\hat{r}) z_2 \rangle. \quad (\text{III.59})$$

Proof of Proposition III.12. We have $Ti = ue^{\hat{r}}i = uie^{-\hat{r}} = iue^{-\hat{r}}$ and for all $z \in \mathcal{Z}$

$$\begin{aligned} \text{Tr}[\rho W(-i\sqrt{2}z)] &= \text{Tr}[\mathbb{U}_T^* \Omega \Omega^* \mathbb{U}_T W(-i\sqrt{2}z)] \\ &= \Omega^* W(ue^{\hat{r}}(-i\sqrt{2}z)) \Omega \\ &= \Omega^* W(-i\sqrt{2}ue^{-\hat{r}}z) \Omega \\ &= \exp\left(-\frac{1}{2}|ue^{-\hat{r}}z|^2\right) \\ &= \exp\left(-\frac{1}{2}|e^{-\hat{r}}z|^2\right) \end{aligned}$$

From this formula we can easily compute the function

$$h(t, s) := \text{Tr}[\rho W(-ti\sqrt{2}z)W(-si\sqrt{2}z)] = \exp\left(-\frac{1}{2}|e^{-\hat{r}}(t+s)z|^2\right)$$

whose derivative $\partial_t \partial_s$ at $(t, s) = (0, 0)$ involves α and γ

$$\begin{aligned}\partial_t \partial_s h(0, 0) &= \text{Tr}[\rho(a^*(z) - a(z))^2] \\ &= -2z^* \gamma z + 2\text{Re}(\alpha^* z^{\vee 2}) - z^* z.\end{aligned}$$

But we have also

$$\begin{aligned}\partial_t \partial_s \exp\left(-\frac{1}{2}|e^{-\hat{r}}(t+s)z|^2\right)\Big|_{t=s=0} &= -(e^{-\hat{r}}z)^*(e^{-\hat{r}}z) \\ &= -(\cosh(\hat{r})z - \sinh(\hat{r})z)^*(\cosh(\hat{r})z - \sinh(\hat{r})z) \\ &= -(\cosh(\hat{r})z)^*(\cosh(\hat{r})z) \\ &\quad + 2\text{Re}(\sinh(\hat{r})z)^*(\cosh(\hat{r})z) - (\sinh(\hat{r})z)^*(\sinh(\hat{r})z) \\ &= -z^*(\cosh^2 \hat{r} + \sinh^2 \hat{r})z + 2\text{Re}(z^*(\sinh \hat{r} \cosh \hat{r})z) \\ &= -z^* \cosh(2\hat{r})z + 2\text{Re}(z^* \frac{1}{2} \sinh(2\hat{r})z)\end{aligned}$$

and hence, using the polarization identity

$$4z \vee z' = (z + z')^{\otimes 2} - (z - z')^{\otimes 2}$$

to recover every vector from $\mathcal{Z}^{\vee 2}$ from linear combinations of vectors of the form $z^{\vee 2}$, we arrive at (III.58)-(III.59). \square

Proposition III.13. *The admissible γ , α for a pure quasifree state are exactly those satisfying the relation*

$$\gamma + \gamma^2 = (\alpha \otimes \mathbf{1})^*(\mathbf{1} \otimes \alpha), \quad (\text{III.60})$$

with $\gamma \geq 0$.

This is the constraint when we minimize the energy as a function of (f, γ, α) with the method of Lagrange multipliers in Section VIII.

Proof. If γ, α are associated with a quasifree state, then there is an \hat{r} such that γ, α and \hat{r} satisfy Equations (III.58) and (III.59), then

$$\begin{aligned}\langle z_1, (\alpha^* \otimes \mathbf{1})(\mathbf{1} \otimes \alpha)z_2 \rangle &= (\alpha^* \otimes z_1^*)(z_2 \otimes \alpha) \\ &= ([\alpha^*(z_2 \otimes \mathbf{1})] \otimes z_1^*)\alpha \\ &= \langle \alpha^*(z_2 \otimes \mathbf{1}), \frac{1}{2} \sinh(2\hat{r})z_1 \rangle_{\mathcal{Z}} \\ &= \langle \alpha^*, z_2 \otimes \frac{1}{2} \sinh(2\hat{r})z_1 \rangle_{\mathcal{Z}^{\otimes 2}} \\ &= \langle \frac{1}{4} \sinh^2(2\hat{r})z_1, z_2 \rangle_{\mathcal{Z}} \\ &= \langle (\frac{1}{2}(\cosh(2\hat{r}) - \mathbf{1}) + \frac{1}{4}(\cosh(2\hat{r}) - \mathbf{1})^2)z_1, z_2 \rangle_{\mathcal{Z}}.\end{aligned}$$

Conversely, if γ and α satisfy Eq. (III.60) then we define the \mathbb{C} -antilinear operator $\hat{\alpha}$ such that $\langle z_1, \hat{\alpha} z_2 \rangle = (z_1 \otimes z_2)^* \alpha$, and set $\hat{r} = \frac{1}{2} \sinh^{-1}(2\hat{\alpha})$, then

$$\forall z_1, z_2 \in \mathcal{Z} : \quad \langle z_1 \otimes z_2, \alpha_\rho \rangle_{\mathcal{Z}^2} = \langle z_1, \hat{\alpha} z_2 \rangle = \langle z_1, \frac{1}{2} \sinh(2\hat{r}) z_2 \rangle,$$

which, in turn, implies that $(\alpha^* \otimes \mathbf{1})(\mathbf{1} \otimes \alpha) = \frac{1}{4} \sinh^2(2\hat{r})$. Hence, we have

$$\gamma + \gamma^2 = \frac{1}{4} \sinh^2(2\hat{r})$$

and as $\gamma \geq 0$, it follows that $\gamma = \frac{1}{2}(\cosh(2\hat{r}) - 1)$. Then γ, α is associated with the centered pure quasifree state whose symplectic transformation is $\exp[\hat{r}]$. \square

IV Energy Functional

Notation: We first recall that, as before, we denote by \vec{k} , and $|\vec{k}|$ the multiplication operators $\vec{k} \otimes \mathbf{1}_{\mathbb{C}^2}$ and $|\vec{k}| \otimes \mathbf{1}_{\mathbb{C}^2}$ on $\mathcal{Z} = L^2(S_{\sigma, \Lambda} \times \mathbb{Z}_2)$, with three components in the case of \vec{k} .

We now work at fixed values of total momentum $\vec{p} \in \mathbb{R}^3$. The operator $H_{g, \vec{p}}$ is given by

$$H_{g, \vec{p}} = \frac{1}{2} (d\Gamma(\vec{k}) + 2\text{Re } a^*(\vec{G}) - \vec{p})^2 + d\Gamma(|\vec{k}|),$$

where $\vec{G}(k) = \vec{G}(\vec{k}, \pm) := g|\vec{k}|^{-1/2} \vec{\varepsilon}_\pm(\vec{k})$. The energy of a pure quasifree state ρ associated with $f \in \mathcal{Z}, \gamma \in \mathcal{L}^1(\mathcal{Z}), \alpha \in \mathcal{Z}^{\vee 2}$ is

$$\mathcal{E}_{g, \vec{p}}(f, \gamma, \alpha) := \text{Tr}[H_{g, \vec{p}} \rho], \quad (\text{IV.61})$$

where \mathcal{Z} is the \mathbb{C} -Hilbert space $\mathcal{Z} = L^2(S_{\sigma, \Lambda} \times \mathbb{Z}_2)$ and $\mathcal{L}^1(\mathcal{Z})$ is the space of trace class operators on \mathcal{Z} .

Proposition IV.1. *The energy functional (IV.61) is*

$$\begin{aligned} \mathcal{E}_{g, \vec{p}}(f, \gamma, \alpha) = & \frac{1}{2} \left\{ (\text{Tr}[\gamma \vec{k}] + f^* \vec{k} f + 2\text{Re}(f^* \vec{G}) - \vec{p})^2 \right. \\ & + \text{Tr}[\gamma \vec{k} \cdot \gamma \vec{k}] + \alpha^*(\vec{k} \cdot \otimes \vec{k}) \alpha + \text{Tr}[|\vec{k}|^2 \gamma] \\ & + 2\text{Re}\{\alpha^*[(\vec{G} + \vec{k} f)^{\vee 2}]\} + \text{Tr}[(2\gamma + \mathbf{1})(\vec{G} + \vec{k} f) \cdot (\vec{G} + \vec{k} f)^*] \} \\ & \left. + \text{Tr}[\gamma |\vec{k}|] + f^* |\vec{k}| f \right\}. \end{aligned} \quad (\text{IV.62})$$

where the following positivity properties hold

$$\begin{aligned}
& (\text{Tr}[\gamma \vec{k}] + f^* \vec{k} f + 2\text{Re}(f^* \vec{G}) - \vec{p})^2 \geq 0, \\
& \text{Tr}[\gamma \vec{k} \cdot \gamma \vec{k}] + \text{Tr}[\gamma \vec{k}]^2 + \alpha^*(\vec{k} \cdot \otimes \vec{k})\alpha + \text{Tr}[|\vec{k}|^2 \gamma] \geq 0, \\
& (\text{Tr}[\gamma \vec{k}] + f^* \vec{k} f + 2\text{Re}(f^* \vec{G}) - \vec{p})^2 \\
& + \text{Tr}[\gamma \vec{k} \cdot \gamma \vec{k}] + \alpha^*(\vec{k} \cdot \otimes \vec{k})\alpha + \text{Tr}[|\vec{k}|^2 \gamma] \geq 0, \\
& 2\text{Re}(\alpha^*((\vec{G} + \vec{k}f)^{\vee 2})) + \text{Tr}[(2\gamma + \mathbf{1})(\vec{G} + \vec{k}f) \cdot (\vec{G} + \vec{k}f)^*] \geq 0.
\end{aligned}$$

The energy of a pure quasifree state in the variables f and \hat{r} is

$$\begin{aligned}
\hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r}) = & \frac{1}{2} \{ (\text{Tr}[\frac{1}{2}(\cosh(2\hat{r}) - 1)\vec{k}] + f^* \vec{k} f + 2\text{Re}(f^* \vec{G}) - \vec{p})^2 \\
& + \text{Tr}[\frac{1}{2}(\cosh(2\hat{r}) - 1)\vec{k} \cdot \frac{1}{2}(\cosh(2\hat{r}) - 1)\vec{k}] \\
& + \text{Tr}[\frac{1}{2}\sinh(2\hat{r})\vec{k} \cdot \frac{1}{2}\sinh(2\hat{r})\vec{k}] + \text{Tr}[|\vec{k}|^2 \frac{1}{2}(\cosh(2\hat{r}) - 1)] \\
& + 2\text{Re}(\frac{1}{2}\sinh(2\hat{r})(\vec{G} + \vec{k}f); (\vec{G} + \vec{k}f)) \\
& + \text{Tr}[(2\frac{1}{2}(\cosh(2\hat{r}) - 1) + \mathbf{1})(\vec{G} + \vec{k}f) \cdot (\vec{G} + \vec{k}f)^*] \} \\
& + \text{Tr}[\frac{1}{2}(\cosh(2\hat{r}) - 1)|\vec{k}|] + f^* |\vec{k}| f. \tag{IV.63}
\end{aligned}$$

Proof. Using the Weyl operators,

$$\mathcal{E}_{g,\vec{p}}(f, \gamma, \alpha) := \text{Tr}[H_{g,\vec{p}}\rho] = \text{Tr}[H_{g,\vec{p}}(f)\tilde{\rho}]$$

where $H_{g,\vec{p}}(f) = W(\sqrt{2}f/i)^* H_{g,\vec{p}} W(\sqrt{2}f/i)$ and $\tilde{\rho} = W(\sqrt{2}f/i)^* \rho W(\sqrt{2}f/i)$, so that $\tilde{\rho}$ is centered. Modulo terms of odd order, which vanish when we take the trace against a centered quasifree state, $H_{g,\vec{p}}(f)$ equals

$$\begin{aligned}
H_{g,\vec{p}}(f) = & \frac{1}{2} (d\Gamma(\vec{k}) + f^* \vec{k} f + 2\text{Re}(a^*(\vec{k}f + \vec{G})) + 2\text{Re}(f^* \vec{G}) - \vec{p})^2 \\
& + d\Gamma(|\vec{k}|) + f^* |\vec{k}| f + \text{odd} \\
= & \frac{1}{2} (d\Gamma(\vec{k}) + f^* \vec{k} f + 2\text{Re}(f^* \vec{G}) - \vec{p})^2 \\
& + \frac{1}{2} (2\text{Re}(a^*(\vec{k}f + \vec{G})))^2 + d\Gamma(|\vec{k}|) + f^* |\vec{k}| f + \text{odd}.
\end{aligned}$$

To compute $\mathcal{E}(f, \gamma, \alpha)$ we are thus lead to compute, for $\vec{\varphi} \in \mathcal{Z}^3$ and $\vec{u} \in \mathbb{R}^3$,

$$\text{Tr}[\tilde{\rho}(d\Gamma(\vec{k}) + \vec{u})^2] \quad \text{and} \quad \text{Tr}[\tilde{\rho}(2\text{Re}\{a(\vec{\varphi})\})^2].$$

The expression of the energy as a function of (f, γ, α) then follows from Propositions IV.2 and IV.4. The expression of the energy as a function of (f, r) follows from Proposition III.12. \square

Proposition IV.2. *Let $\vec{u} \in \mathbb{R}^3$, then*

$$0 \leq \text{Tr}[\tilde{\rho}(d\Gamma(\vec{k}) + \vec{u})^2] = (\text{Tr}[\gamma\vec{k}] + \vec{u})^2 - \text{Tr}[\gamma\vec{k}]^2 \\ + \text{Tr}[\gamma\vec{k} \cdot \gamma\vec{k}] + \text{Tr}[\gamma\vec{k}]^2 + \alpha^*(\vec{k} \cdot \otimes \vec{k})\alpha + \text{Tr}[|\vec{k}|^2\gamma].$$

This condition is used with $\vec{u} = \vec{p} - f^*\vec{k}f - 2\text{Re}(f^*\vec{G})$.

Proof. Indeed,

$$(d\Gamma(\vec{k}) + \vec{u})^2 = d\Gamma(\vec{k})^2 + 2d\Gamma(\vec{k}) \cdot \vec{u} + \vec{u}^2.$$

Then we use that $\text{Tr}[\tilde{\rho} d\Gamma(\vec{k})] = \text{Tr}[\gamma\vec{k}]$, add and subtract $\text{Tr}[\gamma\vec{k}]^2$ to complete the square and compute $\text{Tr}[\tilde{\rho} d\Gamma(\vec{k})^2]$ using Lemma IV.3. \square

Lemma IV.3. *Let $X \in \mathcal{B}^{1,1}$, then*

$$0 \leq \text{Tr}[\tilde{\rho} d\Gamma(X) d\Gamma(X)^*] = \text{Tr}[\gamma X \gamma X^*] + |\text{Tr}[\gamma X]|^2 + \alpha^*(X \otimes X^*)\alpha + \text{Tr}[X X^* \gamma].$$

Proof. Indeed, using Equation (III.57),

$$\begin{aligned} & \text{Tr}[\tilde{\rho} d\Gamma(X) d\Gamma(X)^*] \\ &= \text{Tr}[\tilde{\rho} \left(\int X(k_1, k'_1) X(k_2, k'_2) a^*(k_1) a^*(k_2) a(k'_2) a(k'_1) dk_1 dk_2 dk'_1 dk'_2 + d\Gamma(X X^*) \right)] \\ &= \text{Tr}[(\gamma \otimes \gamma + \gamma \otimes \gamma E x + \alpha \alpha^*)(X \otimes X^*)] + \text{Tr}[\gamma X X^*] \\ &= \text{Tr}[\gamma X] \text{Tr}[\gamma X^*] + \text{Tr}[\gamma X \gamma X^*] + \alpha^*(X \otimes X^*)\alpha + \text{Tr}[\gamma X X^*]. \end{aligned} \quad \square$$

Proposition IV.4. *Let $\varphi \in \mathcal{Z}$, then*

$$0 \leq \text{Tr}[\tilde{\rho}(a^*(\varphi) + a(\varphi))^2] = 2\text{Re}(\alpha^*(\varphi^{\vee 2})) + \text{Tr}[(2\gamma + \mathbf{1})\varphi\varphi^*] \quad (\text{IV.64})$$

and $|2\text{Re}(\alpha^*(\varphi^{\vee 2}))| \leq \text{Tr}[(2\gamma + \mathbf{1})\varphi\varphi^*]$.

This condition is used with the three components of $\vec{\varphi} = \vec{G} + \vec{k}f$.

Proof. A computation using the canonical commutation relations yields

$$\begin{aligned} & \text{Tr}[\tilde{\rho}(a^*(\varphi) + a(\varphi))^2] \\ &= \text{Tr}[\tilde{\rho}(a^*(\varphi))^2 + \tilde{\rho}(a(\varphi))^2 + \tilde{\rho}(a^*(\varphi)a(\varphi) + a(\varphi)a^*(\varphi))] \\ &= \alpha^*\varphi^{\vee 2} + \varphi^{\vee 2*}\alpha + \text{Tr}[\gamma\varphi\varphi^* + (\gamma + \mathbf{1})\psi\psi^*]. \end{aligned}$$

\square

V Minimization over Coherent States

For this section we can take $\sigma = 0$ if we consider the parameter f in the energy to be in $\tilde{\mathcal{Z}} := L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2, (\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)dk)$. Recall that $S_{\sigma,\Lambda} = \{\vec{k} \in \mathbb{R}^3 \mid \sigma \leq |\vec{k}| \leq \Lambda\}$.

Remark V.1. For a coherent state (see Definition II.4) the energy reduces to

$$\mathcal{E}_{g,\vec{p}}(f) = \frac{1}{2}\|\vec{G}\|^2 + \frac{1}{2}(f^*\vec{k}f + 2\text{Re}(f^*\vec{G}) - \vec{p})^2 + f^*(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)f. \quad (\text{V.65})$$

Note that, for $\sigma > 0$, $\mathcal{Z} = L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2, dk) = \tilde{\mathcal{Z}}$, while for $\sigma = 0$, $\mathcal{Z} \subset \tilde{\mathcal{Z}}$, and $\mathcal{E}_{g,\vec{p}}(f)$ extends to $\tilde{\mathcal{Z}}$ by using Equation (V.65).

Theorem V.2. *There exists a universal constant $C < \infty$ such that, for $0 \leq \sigma < \Lambda < \infty$, $g^2 \ln(\Lambda + 2) \leq C$ and $|\vec{p}| \leq 1/3$, there exists a unique $f_{\vec{p}}$ which minimizes $\mathcal{E}_{g,\vec{p}}$ in $\tilde{\mathcal{Z}}$.*

1. The minimizer $f_{\vec{p}}$ solves the system of equations

$$f_{\vec{p}} = \frac{\vec{u}_{\vec{p}} \cdot \vec{G}}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u}_{\vec{p}}}, \quad (\text{V.66})$$

$$\vec{u}_{\vec{p}} = \vec{p} - 2\text{Re}(f_{\vec{p}}^*\vec{G}) - f_{\vec{p}}^*\vec{k}f_{\vec{p}}, \quad (\text{V.67})$$

with $|\vec{u}_{\vec{p}}| \leq |\vec{p}|$.

2. For $0 \leq \sigma < \Lambda < \infty$,

$$\inf_{f \in \mathcal{Z}} \mathcal{E}_{g,\vec{p}}(f) = \inf_{f \in \tilde{\mathcal{Z}}} \mathcal{E}_{g,\vec{p}}(f) = \mathcal{E}_{g,\vec{p}}(f_{\vec{p}}),$$

and for $0 < \sigma < \Lambda < \infty$, we have that $f_{\vec{p}} \in \mathcal{Z}$.

3. For fixed g, σ, Λ , as a function of \vec{p} ,

$$\mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) = \mathcal{E}_{g,\vec{p}}(0) - \vec{p} \cdot \vec{G}^* \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G} \cdot \vec{G}^*} \vec{G} \cdot \vec{p} + \mathcal{O}(|\vec{p}|^3).$$

4. For all f in $\tilde{\mathcal{Z}}$,

$$\begin{aligned} \mathcal{E}_{g,\vec{p}}(f_{\vec{p}} + f) &= \mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) + f^*(\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{u}_{\vec{p}} \cdot \vec{k})f \\ &\quad + \frac{1}{2}(f^*\vec{k}f + 2\text{Re}(f_{\vec{p}}^*\vec{k}f) + 2\text{Re}(f^*\vec{G}))^2. \end{aligned} \quad (\text{V.68})$$

5. The energy $\mathcal{E}_{g,\vec{p}}(f_{\vec{p}})$ of the minimizer compared to the energy of the vacuum state $\mathcal{E}_{g,\vec{p}}(0)$ is

$$\mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) = \mathcal{E}_{g,\vec{p}}(0) - \frac{1}{2}2\text{Re}(f_{\vec{p}}^* \vec{u}_{\vec{p}} \cdot \vec{G}) - \frac{1}{2}|\vec{u}_{\vec{p}} - \vec{p}|^2.$$

Note that the term $2\text{Re}(f_{\vec{p}}^* \vec{u}_{\vec{p}} \cdot \vec{G})$ is non-negative.

Remark V.3. Our hypotheses are similar those of Chen, Fröhlich, and Pizzo [8], where their vector $\vec{\nabla} E_p^\sigma$ is analogous to $\vec{u}_{\vec{p}}$ in our notations.

The construction of $\vec{u}_{\vec{p}}$ as the solution of a fixed point problem and the dependency in the parameter \vec{p} imply that the map $\vec{p} \mapsto \vec{u}_{\vec{p}}$ is of class \mathcal{C}^∞ .

Remark V.4. We note that we also expect to have $\vec{u}_{\vec{p}}$ in the neighborhood of \vec{p} .

Remark V.5. The minimizer is constructed as the solution of a fixed point problem. As a result the application

$$(\sigma, \Lambda, g, \vec{p}) \mapsto \inf_{\rho \in \text{coh}} \text{Tr}[H_{g,\vec{p}} \rho]$$

is continuous on the domain defined by Theorem V.2, and at σ, Λ fixed,

$$(g, \vec{p}) \mapsto \inf_{\rho \in \text{coh}} \text{Tr}[H_{g,\vec{p}} \rho]$$

is analytic for $g^2 < C/\ln(\Lambda + 2)$ and $|\vec{p}| < 1/3$.

Proof of Theorem V.2. Proof of 1. Assume there is a point $f_{\vec{p}}$ where the minimum is attained. The partial derivative of the energy at the point $f_{\vec{p}}$

$$\begin{aligned} & \partial_{f^*} \mathcal{E}(f_{\vec{p}}) \\ &= ((f_{\vec{p}}^* \vec{k} f_{\vec{p}} - \vec{p} + 2\text{Re}(f_{\vec{p}}^* \vec{G})) \cdot \vec{k} + \frac{1}{2}|\vec{k}|^2 + |\vec{k}|) f_{\vec{p}} - (\vec{p} - f_{\vec{p}}^* \vec{k} f_{\vec{p}} - 2\text{Re}(f_{\vec{p}}^* \vec{G})) \cdot \vec{G} \end{aligned}$$

then vanishes, where the derivative $\partial_{f^*} \mathcal{E}(f)$ at a point f is the unique vector in $\tilde{\mathcal{Z}}^* \cong L^2(S_{\sigma,\Lambda}, (\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)^{-1} dk)$ defined by

$$\mathcal{E}(f + \delta f) - \mathcal{E}(f) = 2\text{Re}(\delta f^* \partial_{f^*} \mathcal{E}(f)) + o(\|\delta f\|_{\tilde{\mathcal{Z}}})$$

with $f, \delta f \in \tilde{\mathcal{Z}}$. Observe that

$$\begin{aligned} 0 &\leq \mathcal{E}_{g,\vec{p}}(0) - \mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) \\ &= \frac{1}{2}|\vec{p}|^2 - \frac{1}{2}(f_{\vec{p}}^* \vec{k} f_{\vec{p}} + 2\text{Re}(f_{\vec{p}}^* \vec{G}) - \vec{p})^2 - f_{\vec{p}}^* (\frac{1}{2}|\vec{k}|^2 + |\vec{k}|) f_{\vec{p}} \end{aligned}$$

and hence $|\vec{p}| \geq |\vec{u}_{\vec{p}}|$ with $\vec{u}_{\vec{p}} := \vec{p} - f_{\vec{p}}^* \vec{k} f_{\vec{p}} - 2\text{Re}(f_{\vec{p}}^* \vec{G})$. Since $|\vec{u}_{\vec{p}}| \leq |\vec{p}| < 1$, it makes sense to write

$$f_{\vec{p}} = \frac{\vec{u}_{\vec{p}} \cdot \vec{G}}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{u}_{\vec{p}} \cdot \vec{k}}.$$

Hence the minimum point $f_{\vec{p}}$ satisfies Equations (V.66) and (V.67). It is in particular sufficient to prove that there exist a unique $\vec{u}_{\vec{p}}$ in a ball $\bar{B}(0, r)$ with $r \geq |\vec{p}|$ such that the function in Equation (V.66) satisfies also Equation (V.67) to prove the existence and uniqueness of a minimizer.

Proof of the existence and uniqueness of a solution. Let $\frac{1}{3} < r < 1$, $\vec{u} \in \mathbb{R}^3$, $|\vec{u}| \leq r < 1$ and

$$\Phi_{\vec{u}}(\vec{k}) = \frac{\vec{u} \cdot \vec{G}(\vec{k})}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u}}.$$

Observe that $\Phi_{\vec{u}} \in \tilde{\mathcal{Z}}$, indeed, if $|\vec{u}| < 1$ then $\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u} \geq (1-r)(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)$, and with $\tilde{\varepsilon}(\vec{k}) = \tilde{\varepsilon}(\vec{k}, +) + \tilde{\varepsilon}(\vec{k}, -)$,

$$\begin{aligned} \int_{|\vec{k}| \in [\sigma, \Lambda]} (\frac{1}{2}|\vec{k}|^2 + |\vec{k}|) |\Phi_{\vec{u}}(\vec{k})|^2 dk &\leq g^2 \int_{|\vec{k}| \in [\sigma, \Lambda]} \frac{1}{|\vec{k}|} \frac{1}{(1-r)^2} \frac{|\vec{u} \cdot \tilde{\varepsilon}(\vec{k})|^2}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} dk < +\infty. \\ &\leq C_0 g^2 \ln(\Lambda + 2) \frac{|\vec{u}|^2}{(1-r)^2} \end{aligned}$$

for some universal constant $C_0 > 0$. Observe then that

$$\int_{|\vec{k}| \in [\sigma, \Lambda]} \frac{|\vec{G}(\vec{k})|^2}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} dk \leq C_0 g^2 \ln(\Lambda + 2)$$

for some universal constant $C_0 > 0$. It follows that $\Phi_{\vec{u}}^* \vec{G} \in L^1(S_{\sigma, \Lambda} \times \mathbb{Z}_2)$. Note that if $\sigma = 0$ then $\Phi_{\vec{u}} \notin L^2(S_{\sigma, \Lambda} \times \mathbb{Z}_2)$ (for $\vec{u} \neq 0$).

We can thus define the application

$$\bar{B}(0, r) \ni \vec{u} \mapsto \vec{\Psi}(\vec{u}) := \vec{p} - \Phi_{\vec{u}}^* \vec{k} \Phi_{\vec{u}} - 2\text{Re}(\Phi_{\vec{u}}^* \vec{G}) \in \mathbb{R}^3.$$

We check that the hypotheses of the Banach-Picard fixed point theorem are verified on the ball $\bar{B}(0, r)$, which will prove the result.

Stability: If $g^2 \ln(\Lambda + 2)$ is sufficiently small, we get from

$$|\vec{\Psi}(\vec{u})| \leq |\Phi_{\vec{u}}^* \vec{k} \Phi_{\vec{u}}| + |2\text{Re}(\Phi_{\vec{u}}^* \vec{G})| + |\vec{p}|$$

and the estimates above that the sum of the two first terms is smaller than $r - 1/3$ and since $|\vec{p}| \leq 1/3$ the map $\vec{\Psi}$ sends $\bar{B}(0, r)$ into itself,

$$\vec{\Psi}(\bar{B}(0, r)) \subseteq \bar{B}(0, r).$$

Contraction: For \vec{u} and \vec{v} in $\bar{B}(0, r)$, we have that

$$\begin{aligned}
& |\Phi_{\vec{u}}(\vec{k}) - \Phi_{\vec{v}}(\vec{k})|(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|) \\
&= \left| \frac{\vec{u} \cdot \vec{G}(\vec{k})}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u}} - \frac{\vec{v} \cdot \vec{G}(\vec{k})}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{v}} \right|(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|) \\
&\leq \left(\frac{|\vec{u} - \vec{v}| |\vec{G}(\vec{k})|}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u}} \right. \\
&\quad \left. + |\vec{v}| |\vec{G}(\vec{k})| \left| \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{v}} - \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u}} \right| \right) (\frac{1}{2}|\vec{k}|^2 + |\vec{k}|) \\
&\leq |\vec{u} - \vec{v}| |\vec{G}(\vec{k})| \frac{1}{(1-r)} \left(1 + \frac{r|\vec{k}|}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|(1-r)} \right) \\
&\leq |\vec{u} - \vec{v}| |\vec{G}(\vec{k})| \frac{1}{(1-r)^2}.
\end{aligned}$$

For the term $2\text{Re}(\Phi_{\vec{u}}^* \vec{G})$, we observe that

$$\begin{aligned}
& |2\text{Re}(\Phi_{\vec{u}}^* \vec{G}) - 2\text{Re}(\Phi_{\vec{v}}^* \vec{G})| \\
&\leq g^2 2|\vec{u} - \vec{v}| \frac{1}{(1-r)^2} \int_{|\vec{k}| \in [\sigma, \Lambda]} \frac{1}{|\vec{k}|} \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} d^3k \\
&\leq C_1 g^2 \ln(2 + \Lambda) 2|\vec{u} - \vec{v}| \frac{1}{(1-r)^2}.
\end{aligned}$$

Note that, for $g^2 \ln(2 + \Lambda) < (1-r)^2/(3C_1)$,

$$|2\text{Re}(\Phi_{\vec{u}}^* \vec{G}) - 2\text{Re}(\Phi_{\vec{v}}^* \vec{G})| < \frac{1}{3} |\vec{u} - \vec{v}|.$$

Finally, for the term $\Phi_{\vec{u}}^* \vec{k} \Phi_{\vec{u}}$, we obtain the estimate

$$\begin{aligned}
& |\Phi_{\vec{u}}^* \vec{k} \Phi_{\vec{u}} - \Phi_{\vec{v}}^* \vec{k} \Phi_{\vec{v}}| \\
&\leq \int_{|\vec{k}| \in [\sigma, \Lambda]} (\frac{1}{2}|\vec{k}|^2 + |\vec{k}|) |\Phi_{\vec{u}}(\vec{k}) - \Phi_{\vec{v}}(\vec{k})| (|\Phi_{\vec{u}}(\vec{k})| + |\Phi_{\vec{v}}(\vec{k})|) d^3k \\
&\leq \frac{|\vec{u} - \vec{v}|}{(1-r)^2} \int_{|\vec{k}| \in [\sigma, \Lambda]} |\vec{G}(\vec{k})| (|\Phi_{\vec{u}}(\vec{k})| + |\Phi_{\vec{v}}(\vec{k})|) d\vec{k} \\
&\leq \frac{|\vec{u} - \vec{v}|}{(1-r)^2} \|(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)^{-1/2} G\| (\|\sqrt{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} \Phi_{\vec{u}}\| + \|\sqrt{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} \Phi_{\vec{v}}\|) \\
&\leq C_2 |\vec{u} - \vec{v}| (|\vec{u}| + |\vec{v}|) g^2 \ln(\Lambda + 2),
\end{aligned}$$

and thus this term can be controlled for $|g \ln(\Lambda + 2)|^2$ sufficiently small by $\frac{1}{3}|\vec{u} - \vec{v}|$. We thus get a contraction

$$|\vec{\Psi}(\vec{u}) - \vec{\Psi}(\vec{u}')| \leq \frac{2}{3}|\vec{u} - \vec{u}'|$$

and with $f_{\vec{p}} = \Phi_{\vec{u}_{\vec{p}}}$ Equation (V.66) is solved.

Proof of 3. The expression of the energy $\mathcal{E}_{g,\vec{p}}(f)$ given in Equation (V.65) implies that $\mathcal{E}_{g,\vec{p}}(f) \geq \frac{1}{2}\|\vec{G}\|^2$, and for $\vec{p} = \vec{0}$ this minimum is only attained at the point $f_{\vec{0}} = 0$. It follows that $f_{\vec{p}} = \partial_{\vec{p}} f_{\vec{0}} \cdot \vec{p} + \mathcal{O}(|\vec{p}|^2)$. From Equation (V.67) we deduce

$$\vec{u}_{\vec{p}} = \vec{p} - 2\text{Re}((\partial_{\vec{p}} f_{\vec{0}} \cdot \vec{p})^* \vec{G}) + \mathcal{O}(|\vec{p}|^2)$$

and thus

$$\begin{aligned} f_{\vec{p}} &= \frac{(\vec{p} - 2\text{Re}((\partial_{\vec{p}} f_{\vec{0}} \cdot \vec{p})^* \vec{G})) \cdot \vec{G}}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u}_{\vec{p}}} + \mathcal{O}(|\vec{p}|^2) \\ &= \left(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|\right)^{-1} (\vec{p} - 2\text{Re}((\partial_{\vec{p}} f_{\vec{0}} \cdot \vec{p})^* \vec{G})) \cdot \vec{G} + \mathcal{O}(|\vec{p}|^2). \end{aligned}$$

Expanding the left hand side of this equality in $\vec{0}$ brings

$$\partial_{\vec{p}} f_{\vec{0}} \cdot \vec{p} = \left(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|\right)^{-1} (\vec{p} - 2\text{Re}((\partial_{\vec{p}} f_{\vec{0}} \cdot \vec{p})^* \vec{G})) \cdot \vec{G}$$

and hence $\partial_{\vec{p}} f_{\vec{0}} = (\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G} \cdot \vec{G}^*)^{-1} \vec{G}$. The expansion of $f_{\vec{p}}$ to the second order is then

$$f_{\vec{p}} = \left(\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G} \cdot \vec{G}^*\right)^{-1} \vec{G} \cdot \vec{p} + \mathcal{O}(|\vec{p}|^2).$$

We can compute the energy modulo error terms in $\mathcal{O}(|\vec{p}|^3)$. To have less heavy computations we set $A = \frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G} \cdot \vec{G}^*$ and get

$$\begin{aligned} \mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) &- \frac{1}{2}\|\vec{G}\|^2 - \frac{1}{2}|\vec{p}|^2 \\ &\equiv -\frac{1}{2}|\vec{p}|^2 + \frac{1}{2}(2\text{Re}(\vec{p} \cdot \partial_{\vec{p}} f_{\vec{0}}^* \vec{G}) - \vec{p} \cdot \vec{p}) + \vec{p} \cdot \partial_{\vec{p}} f_{\vec{0}}^* \left(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|\right) \partial_{\vec{p}} f_{\vec{0}}^* \cdot \vec{p} \\ &\equiv \frac{1}{2}(2\text{Re}(\vec{p} \cdot \vec{G}^* A^{-1} \vec{G}))^2 - 2\vec{p} \cdot \vec{G}^* A^{-1} \vec{G} \cdot \vec{p} \\ &\quad + \vec{p} \cdot \vec{G}^* A^{-1} \left(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|\right) A^{-1} \vec{G} \cdot \vec{p} \\ &\equiv 2(\vec{p} \cdot \vec{G}^* A^{-1} \vec{G})^2 + \vec{p} \cdot \vec{G}^* A^{-1} \left(\left(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|\right) - 2A\right) A^{-1} \vec{G} \cdot \vec{p} \\ &\equiv \vec{p} \cdot \vec{G}^* A^{-1} 2\vec{G} \cdot \vec{G}^* A^{-1} \vec{G} \cdot \vec{p} - \vec{p} \cdot \vec{G}^* A^{-1} \left(\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 4\vec{G} \cdot \vec{G}^*\right) A^{-1} \vec{G} \cdot \vec{p} \\ &\equiv -\vec{p} \cdot \vec{G}^* \left(\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G} \cdot \vec{G}^*\right)^{-1} \vec{G} \cdot \vec{p} \end{aligned}$$

which yields the result.

Proof of 4. The Taylor expansion of the energy around $f_{\vec{p}}$ is

$$\begin{aligned}\mathcal{E}_{g,\vec{p}}(f_{\vec{p}} + f) &= \mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) + f^* \partial_{f^*} \mathcal{E}(f_{\vec{p}}) + \partial_f \mathcal{E}(f_{\vec{p}}) f \\ &\quad + \frac{1}{2} \left\{ (f^* \vec{k} f + 2\operatorname{Re}(f^* \vec{G}) + 2\operatorname{Re}(f_{\vec{p}}^* \vec{k} f))^2 \right. \\ &\quad \left. + 2(f_{\vec{p}}^* \vec{k} f_{\vec{p}} + 2\operatorname{Re}(f_{\vec{p}}^* \vec{G}) - \vec{p}) \cdot f^* \vec{k} f + f^* |\vec{k}|^2 f \right\} + f^* |\vec{k}| f.\end{aligned}$$

Since $\partial_{f^*} \mathcal{E}(f_{\vec{p}})$ vanishes this gives Equation (V.68).

Proof of 5. It is sufficient to replace f by $-f_{\vec{p}}$ in Equation (V.68). The observation

$$f_{\vec{p}}^* \vec{u}_{\vec{p}} \cdot \vec{G} = \int \frac{(\vec{u}_{\vec{p}} \cdot \vec{G}(\vec{k}))^2 dk}{\frac{1}{2} |\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u}_{\vec{p}}}$$

shows that $2\operatorname{Re}(f_{\vec{p}}^* \vec{u}_{\vec{p}} \cdot \vec{G})$ is non-negative since $|\vec{u}_{\vec{p}}| < 1$. \square

VI The Minimizer for the Energy Functional varying over Pure Quasifree States

Definition VI.1. Let \mathcal{Z} be a \mathbb{C} -Hilbert space. Let Y be the \mathbb{R} -Hilbert space of antilinear operators \hat{r} on \mathcal{Z} , self-adjoint in the sense that $\forall z, z' \in \mathcal{Z}$, $\langle z, \hat{r} z' \rangle = \langle z', \hat{r} z \rangle$, and Hilbert-Schmidt in the sense that the positive operator \hat{r}^2 is trace class. The space $X = \mathcal{Z} \times Y$ with the scalar product

$$\langle (f, \hat{r}), (f', \hat{r}') \rangle_X = f^* f' + \operatorname{Tr}[\hat{r} \hat{r}']$$

is an \mathbb{R} -Hilbert space.

Keeping $\sigma > 0$, we only need to use $\mathcal{Z} = L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2)$ in this section.

Theorem VI.2. *Let $0 < \sigma < \Lambda < \infty$. There exists $C > 0$ such that for $g, |\vec{p}| \leq C$ there exists a unique minimizer for $\hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r})$.*

Proof. This result follows from convexity and coercivity arguments. By Proposition VI.3, $\hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r})$ is strictly θ -convex (i.e., uniformly strictly convex) on $\bar{B}_X(0, R)$ for some $R > 0$ and $\theta > 0$. Since $\hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r})$ is strongly continuous on the closed and convex set $\bar{B}_X(0, R)$ of the Hilbert space X we get the existence and uniqueness of a minimizer in $\bar{B}_X(0, R)$. (See for example [1]. The uniform strict convexity allows to prove directly that a minimizing sequence is a Cauchy sequence.) Proposition VI.4 then proves that it is the only minimum of $\hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r})$ on the whole space.

Note that to use Propositions VI.3 and VI.4 we need to restrict to values of g and $|\vec{p}|$ smaller than some constant $C > 0$. \square

Proposition VI.3 (Convexity). *There exist $0 < C, R < \infty$ such that for $g \leq C$ and $|\vec{p}| \leq \frac{1}{2}$, the Hessian of the energy satisfies $\mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r}) \geq \frac{\sigma}{4}\mathbf{1}_X$ on the ball $B_X(0, R)$.*

Proof. We use that strict positivity of the Hessian implies strict convexity and thus first compute the Hessian in $(0, 0)$. The Hessian $\mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r}) \in \mathcal{B}(X)$ is defined using the Fréchet derivative

$$\begin{aligned} & \hat{\mathcal{E}}_{g,\vec{p}}(f + \delta f, \hat{r} + \delta \hat{r}) - \hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r}) \\ &= D\hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r})(\delta f, \delta \hat{r}) + \frac{1}{2}\langle (\delta f, \delta \hat{r}), \mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r})(\delta f, \delta \hat{r}) \rangle_X + o(\|(\delta f, \delta \hat{r})\|_X^2) \end{aligned}$$

with $D\hat{\mathcal{E}}_{g,\vec{p}}(0, 0) \in \mathcal{B}(X, \mathbb{R})$. (Note that differentiability is granted in this case because $|\vec{k}| \leq \Lambda < \infty$.) For any $\mu > 0, \forall (f, \hat{r}) \in X$,

$$\begin{aligned} & \langle (f, \hat{r}), \frac{1}{2}\mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(0, 0)(f, \hat{r}) \rangle_X \\ &= 2\text{Re}\langle \hat{r}\vec{k}f; \vec{G} \rangle + \frac{1}{2}(2\text{Re}(f^*\vec{G}))^2 + \text{Tr}[\hat{r}^2\vec{G} \cdot \vec{G}^*] \\ & \quad + \frac{1}{2}\{\text{Tr}[\hat{r}\vec{k} \cdot \hat{r}\vec{k}] + \text{Tr}[|\vec{k}|^2\hat{r}^2]\} \\ & \quad + \text{Tr}[\hat{r}^2(|\vec{k}| - \vec{k} \cdot \vec{p})] + f^*(\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{p})f \\ &\geq \text{Tr}[\hat{r}^2\vec{G} \cdot \vec{G}^*] - \mu\|\hat{r}\vec{G}\|^2 - \frac{1}{\mu}\|\vec{k}f\|^2 \\ & \quad + \frac{1}{2}\{(2\text{Re}(\delta f^*\vec{G}))^2 + \text{Tr}[\hat{r}\vec{k} \cdot \hat{r}\vec{k}] + \text{Tr}[|\vec{k}|^2\hat{r}^2]\} \\ & \quad + \text{Tr}[\hat{r}^2(|\vec{k}| - \vec{k} \cdot \vec{p})] + f^*(\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{p})f \\ &\geq \text{Tr}[\hat{r}^2(|\vec{k}| - \vec{k} \cdot \vec{p} + (1 - \mu)\vec{G} \cdot \vec{G}^*)] + f^*((\frac{1}{2} - \frac{1}{\mu})|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{p})f, \end{aligned}$$

since

$$|2\text{Re}\langle \hat{r}\vec{k}f; \vec{G} \rangle| \leq 2\|\hat{r}\vec{G}\|\|\vec{k}f\| = 2\sqrt{\mu}\|\hat{r}\vec{G}\|\frac{1}{\sqrt{\mu}}\|\vec{k}f\| \leq \mu\|\hat{r}\vec{G}\|^2 + \frac{1}{\mu}\|\vec{k}f\|^2.$$

With $\mu = 2$ we obtain (with $|\vec{p}| \leq \frac{1}{2}$)

$$\begin{aligned} \frac{1}{2}\mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(0, 0)(f, \hat{r}) &\geq \text{Tr}[\hat{r}^2(|\vec{k}| - \vec{k} \cdot \vec{p} - \vec{G} \cdot \vec{G}^*)] + f^*(|\vec{k}| - \vec{k} \cdot \vec{p})f \\ &\geq \text{Tr}[\hat{r}^2(|\vec{k}|(1 - \|\vec{k}\|^{-1/2}\|\vec{G}\|^2) - \vec{k} \cdot \vec{p})] + f^*(|\vec{k}| - \vec{k} \cdot \vec{p})f \\ &\geq \text{Tr}[\hat{r}^2\sigma(\frac{1}{2} - \|\vec{k}\|^{-1/2}\|\vec{G}\|^2)] + f^*\frac{\sigma}{2}f \end{aligned}$$

and for g small enough

$$\frac{1}{2}\mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(0,0) \geq \frac{\sigma}{4}.$$

We then compare it with the Hessian in points near zero. Observing that the Hessian is continuous with respect to (f, \hat{r}, \vec{p}, g) , we deduce that there exist $R < \infty$ and $C > 0$, as asserted. \square

Proposition VI.4 (Coercivity). *Suppose \vec{p} and $C > 0$ are fixed such that $\frac{1}{2}|\vec{p}|^2 + \frac{1}{2}\|\vec{G}\|^2 < \sigma R^2$, with the value of R given by Proposition VI.3, for any $0 < g < C$. For every $(f, \hat{r}) \in X$,*

$$\hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r}) \geq \text{Tr}[\hat{r}^2|\vec{k}|] + f^*|\vec{k}|f \geq \sigma \|(f, \hat{r})\|_X^2.$$

Since $\hat{\mathcal{E}}_{g,\vec{p}}(0,0) = \frac{1}{2}|\vec{p}|^2 + \frac{1}{2}\|\vec{G}\|^2 < \sigma R^2$, any minimizing sequence takes its values in $\bar{B}_X(0, R)$.

VII Asymptotics for small Coupling and Momentum

We use below an identification between self-adjoint \mathbb{C} -antilinear Hilbert-Schmidt operator \hat{r} and symmetric two vector r given by the relation $\langle \varphi, \hat{r}\psi \rangle_{\mathcal{Z}} = \langle \varphi \otimes \psi, r \rangle_{\mathcal{Z} \otimes 2}$. Note that the self-adjointness condition for \hat{r} is equivalent to the symmetry condition $r \in \mathcal{Z}^{\vee 2}$.

Theorem VII.1. *Let $0 < \sigma < \Lambda < \infty$. There exists $C > 0$ such that for $|g|, |\vec{p}| < C$, there exist two functions $f_{g,\vec{p}}$ and $\hat{r}_{g,\vec{p}}$ which are smooth in (g, \vec{p}) such that the minimum of the energy $\hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r})$ is attained at $(f_{g,\vec{p}}, \hat{r}_{g,\vec{p}})$. These functions satisfy*

$$\begin{aligned} f_{g,\vec{p}} &= \frac{\vec{p} \cdot \vec{G}}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} + \mathcal{O}(\|(g, \vec{p})\|^3) \\ r_{g,\vec{p}} &= -S^{-1}\vec{G} \cdot \vee \vec{G} + \mathcal{O}(\|(g, \vec{p})\|^3), \end{aligned}$$

with $S = \vec{k} \cdot \otimes \vec{k} + 2(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|) \vee \mathbf{1}_{\mathcal{Z}}$. As a consequence

$$\begin{aligned} E_{BHF}(g, \vec{p}, \sigma, \Lambda) \\ = \hat{\mathcal{E}}_{g,\vec{p}}(0_X) - \vec{p} \cdot \vec{G}^* \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} \vec{G} \cdot \vec{p} - \frac{1}{2} \vec{G}^{\vee 2*} S^{-1} \vec{G}^{\vee 2} + \mathcal{O}(\|(g, \vec{p})\|^5). \end{aligned}$$

Remark VII.2. The energy in 0_X is the energy of the vacuum state and is $\hat{\mathcal{E}}_{g,\vec{p}}(0_X) = \frac{1}{2}\vec{p}^2 + \frac{1}{2}\|\vec{G}\|^2$. Further note that

$$(\vec{p} \cdot \vec{G}^*) \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} (\vec{G} \cdot \vec{p}) = g^2 |\vec{p}|^2 \left(2\pi^2 - \frac{8\pi}{3} \right) \ln \left(\frac{\Lambda + 2}{\sigma + 2} \right)$$

and in particular does not depend on the choice of the polarization vectors $\vec{\varepsilon}$.

The quantity $\vec{G}^{\cdot \vee 2*} S^{-1} \vec{G}^{\cdot \vee 2}$ does not depend on the choice of the vectors $\vec{\varepsilon}$ either since

$$\vec{G}^{\cdot \vee 2*} S^{-1} \vec{G}^{\cdot \vee 2} = \sum_{\mu, \nu = \pm} \int \frac{|\vec{\varepsilon}(\vec{k}_1, \mu) \cdot \vec{\varepsilon}(\vec{k}_2, \nu)|^2}{\sqrt{|\vec{k}_1| |\vec{k}_2|} S(\vec{k}_1, \vec{k}_2)} d^3 k_1 d^3 k_2$$

and with $P_{\vec{u}}$ is the orthogonal projection on \vec{u} in \mathbb{R}^3 ,

$$\begin{aligned} \sum_{\mu, \nu = \pm} |\vec{\varepsilon}(\vec{k}_1, \mu) \cdot \vec{\varepsilon}(\vec{k}_2, \nu)|^2 &= \sum_{\mu, \nu = \pm} \text{Tr}_{\mathbb{R}^3} [P_{\vec{\varepsilon}(\vec{k}_1, \mu)} P_{\vec{\varepsilon}(\vec{k}_2, \nu)}] \\ &= \text{Tr}_{\mathbb{R}^3} [P_{\vec{k}_1}^\perp P_{\vec{k}_2}^\perp] \\ &= 1 + \left(\frac{\vec{k}_1}{|\vec{k}_1|} \cdot \frac{\vec{k}_2}{|\vec{k}_2|} \right)^2. \end{aligned}$$

Proof of Theorem VII.1. Let

$$F : (g, \vec{p}, f, \hat{r}) \mapsto \partial_{f, \hat{r}} \hat{\mathcal{E}}_{g, \vec{p}}(f, \hat{r})$$

and $\begin{pmatrix} f \\ \hat{r} \end{pmatrix} (g, \vec{p}) := \begin{pmatrix} f(g, \vec{p}) \\ \hat{r}(g, \vec{p}) \end{pmatrix}$ such that

$$F(g, \vec{p}, \begin{pmatrix} f \\ \hat{r} \end{pmatrix} (g, \vec{p})) = 0, \quad (\text{VII.69})$$

then a derivation of Equation (VII.69) with respect to (f, \hat{r}) brings

$$\partial_{g, \vec{p}} \begin{pmatrix} f \\ \hat{r} \end{pmatrix} (0_{g, \vec{p}}) = - [\partial_{f, \hat{r}} F(0_{g, \vec{p}}, 0_{f, \hat{r}})]^{-1} \partial_{g, \vec{p}} F(0_{g, \vec{p}}, 0_{f, \hat{r}}).$$

The term which is independent of (g, \vec{p}) and quadratic in $\begin{pmatrix} f \\ \hat{r} \end{pmatrix}$ in the energy is

$$\frac{1}{2} \{ \text{Tr}[\hat{r} S \hat{r}] + f^* (|\vec{k}|^2 + 2|\vec{k}|) f \}$$

thus, in $(0_{g, \vec{p}}, 0_{f, \hat{r}})$,

$$\partial_{f, \hat{r}} F = \begin{pmatrix} |\vec{k}|^2 + 2|\vec{k}| & 0 \\ 0 & S \end{pmatrix}.$$

To compute $\partial_{g,\vec{p}}F$ in 0, observe that no part in the energy is linear in (g, \vec{p}) and linear in (f, \hat{r}) . Thus $\partial_{g,\vec{p}}F(0_{g,\vec{p}}, 0_{f,\hat{r}}) = 0$ and we get

$$\partial_{g,\vec{p}}f(0_{g,\vec{p}}) = 0.$$

Differentiating a second time Equation (VII.69) brings

$$0 = \partial_{g,\vec{p}}^2 F + 2\partial_{f,\hat{r}}\partial_{g,\vec{p}}F \circ \partial_{g,\vec{p}}\left(\frac{f}{\hat{r}}\right) + \partial_{f,\hat{r}}F \circ \partial_{g,\vec{p}}^2\left(\frac{f}{\hat{r}}\right) + \partial_{f,\hat{r}}^2 F(\partial_{g,\vec{p}}\left(\frac{f}{\hat{r}}\right), \partial_{g,\vec{p}}\left(\frac{f}{\hat{r}}\right)).$$

Since $\partial_{g,\vec{p}}\left(\frac{f}{\hat{r}}\right)(0_{g,\vec{p}}) = 0$, it follows that

$$\partial_{g,\vec{p}}^2\left(\frac{f}{\hat{r}}\right)(0_{g,\vec{p}}) = -[\partial_{f,\hat{r}}F(0_{g,\vec{p}}, 0_{f,\hat{r}})]^{-1}\partial_{g,\vec{p}}^2 F(0_{g,\vec{p}}, 0_{f,\hat{r}}).$$

The part of the energy which is quadratic in (g, \vec{p}) and linear in (f, \hat{r}) is $-2\text{Re}(f^*\vec{G}) \cdot \vec{p} + \text{Re}\langle \hat{r}\vec{G}; \vec{G} \rangle$, it follows that, in $(0_{g,\vec{p}}, 0_{f,\hat{r}})$,

$$\partial_{g,\vec{p}}^2 F = 2 \left(\begin{pmatrix} 1 & 0 \\ \partial_g \vec{G} & 0 \end{pmatrix} \vee \begin{pmatrix} 0 & -2\partial_g \vec{G} \\ \partial_g \vec{G} & 0 \end{pmatrix} \right),$$

which gives in $0_{g,\vec{p}}$

$$\partial_{g,\vec{p}}^2\left(\frac{f}{\hat{r}}\right) = 2 \left(\begin{pmatrix} 1 & 0 \\ -S^{-1}(\partial_g \vec{G} & 0) \end{pmatrix} \vee \begin{pmatrix} 0 & \frac{\partial_g \vec{G}}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} \\ \partial_g \vec{G} & 0 \end{pmatrix} \right).$$

Hence the expansion of $\left(\frac{f}{\hat{r}}\right)$ up to order 2.

We can thus express the energy around $0_{g,\vec{p}}$ modulo error terms in $\mathcal{O}(\|(g, \vec{p})\|^5)$

$$\begin{aligned} & \min_{f,\hat{r}} \hat{\mathcal{E}}_{g,\vec{p}}(f, \hat{r}) - \hat{\mathcal{E}}_{g,\vec{p}}(0, 0) \\ & \equiv \frac{1}{2} \left\{ (\text{Tr}[\hat{r}^2 \vec{k}] + f^* \vec{k} f + 2\text{Re}(f^* \vec{G}) - \vec{p})^2 + \text{Tr}[\hat{r} \vec{k} \cdot \hat{r} \vec{k}] + \text{Tr}[|\vec{k}|^2 \hat{r}^2] \right. \\ & \quad + 2\text{Re}\langle \hat{r}(\vec{G} + \vec{k}f); (\vec{G} + \vec{k}f) \rangle + \|\vec{G}\|^2 + f^* |\vec{k}|^2 f \} \\ & \quad + \text{Tr}[\hat{r}^2 |\vec{k}|] + f^* |\vec{k}| f - \hat{\mathcal{E}}_{g,\vec{p}}(0, 0) \\ & \equiv -2\text{Re}(f^* \vec{G}) \cdot \vec{p} + \frac{1}{2} \text{Tr}[\hat{r} S \hat{r}] + \text{Re}\langle \hat{r} \vec{G}; \vec{G} \rangle + f^* \left(\frac{1}{2} |\vec{k}|^2 + |\vec{k}| \right) f \\ & \equiv -2\text{Re}(f^* \vec{p} \cdot \vec{G}) + \frac{1}{2} \text{Tr}[\hat{r} S \hat{r}] + \text{Re}\langle \hat{r} \vec{G}; \vec{G} \rangle + f^* \left(\frac{1}{2} |\vec{k}|^2 + |\vec{k}| \right) f \\ & \equiv -2 \frac{(\vec{p} \cdot \vec{G})^* (\vec{p} \cdot \vec{G})}{\frac{1}{2} |\vec{k}|^2 + |\vec{k}|} + \frac{1}{2} \vec{G}^{\cdot \vee 2*} S^{-1} \vec{G}^{\cdot \vee 2} - \vec{G}^{\cdot \vee 2*} S^{-1} \vec{G}^{\cdot \vee 2} + \frac{(\vec{p} \cdot \vec{G})^* (\vec{p} \cdot \vec{G})}{\frac{1}{2} |\vec{k}|^2 + |\vec{k}|} \end{aligned}$$

which completes the proof. \square

VIII Lagrange Equations

This section formulates the results of Section VI in terms of γ and α subject to the constraints $\gamma + \gamma^2 = (\alpha^* \otimes \mathbf{1}_{\mathcal{Z}})(\mathbf{1}_{\mathcal{Z}} \otimes \alpha)$, without reference to the parametrization of γ and α in terms of \hat{r} .

Suppose $f \in \mathcal{Z}$, $\alpha \in \mathcal{Z}^{\vee 2}$, $\gamma \in \mathcal{L}^1(\mathcal{Z})$, $\lambda \in \mathcal{B}(\mathcal{Z}) = \mathcal{B}$ and $\vec{u} \in \mathbb{R}^3$. Let $\mathcal{A}(\lambda) = \frac{1}{2}\vec{k} \cdot \vee \vec{k} + \lambda \vee \mathbf{1}$ and $\mathcal{G}(\gamma) = \gamma + \gamma^2$.

Theorem VIII.1. *Suppose (f, γ, α) is a minimum of the energy functional \mathcal{E} such that $\|\gamma\|_{\mathcal{B}(\mathcal{Z})} < \frac{1}{2}$. Then there is a unique (λ, \vec{u}) such that $(f, \gamma, \alpha, \lambda, \vec{u})$ satisfies the following equations, equivalent to Lagrange equations*

$$M(\gamma, \vec{u})f = -(\vec{k}(\gamma + \frac{1}{2}\mathbf{1}) - \vec{u}) \cdot \vec{G} - \vec{k} \cdot \vee (\vec{G} + \vec{k}f)^* \alpha \quad (\text{VIII.70})$$

$$\mathcal{A}(\lambda)\alpha = -\frac{1}{2}(\vec{G} + \vec{k}f)^{\cdot \vee 2} \quad (\text{VIII.71})$$

$$\gamma = \mathcal{G}^{-1}((\alpha^* \otimes \mathbf{1}_{\mathcal{Z}})(\mathbf{1}_{\mathcal{Z}} \otimes \alpha)) \quad (\text{VIII.72})$$

$$\lambda = \int_0^\infty e^{-t(\frac{1}{2}+\gamma)} (M(\gamma, \vec{u}) + (\vec{G} + \vec{k}f) \cdot (\vec{G} + \vec{k}f)^*) e^{-t(\frac{1}{2}+\gamma)} dt \quad (\text{VIII.73})$$

$$\vec{u} = \vec{p} - \text{Tr}[\gamma \vec{k}] - f^* \vec{k} f - 2\text{Re}(f^* \vec{G}) \quad (\text{VIII.74})$$

with $M(\gamma, \vec{u}) = \frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u} + \vec{k} \cdot \gamma \vec{k}$.

Assuming $|\vec{p}| < \frac{1}{2}$, sufficient conditions such that $M(\gamma, \vec{u})$ and $\mathcal{A}(\lambda)$ are invertible operators are $|\vec{u}| < 1/2$, $\gamma \geq 0$ and $\|\lambda - (|\vec{k}|^2/2 + |\vec{k}| - \vec{p} \cdot \vec{k})\|_{\mathcal{B}} < \sigma/2$. Equations (VIII.70) to (VIII.74) then form a system of coupled explicit equations.

Remark VIII.2. To prove that Equations (VIII.70) to (VIII.74) admit a solution we use here the result of existence of a minimizer proved in Section VI. It can also be proved directly by a fixed point argument by defining the applications

$$\begin{aligned} \Psi_f(f, \alpha, \gamma, \vec{u}) &= -M(\gamma, \vec{u})^{-1}(\vec{k}(\gamma + \frac{1}{2}\mathbf{1}) - \vec{u}) \cdot \vec{G} - \vec{k} \cdot \vee (\vec{G} + \vec{k}f)^* \alpha \\ \Psi_\alpha(f, \lambda) &= -\mathcal{A}(\lambda)^{-1} \frac{1}{2}(\vec{G} + \vec{k}f)^{\cdot \vee 2} \\ \Psi_\gamma(\alpha) &= \mathcal{G}^{-1}((\alpha^* \otimes \mathbf{1}_{\mathcal{Z}})(\mathbf{1}_{\mathcal{Z}} \otimes \alpha)) \\ \Psi_\lambda(f, \gamma, \vec{u}) &= \int_0^\infty e^{-t(\frac{1}{2}+\gamma)} (M(\gamma, \vec{u}) + (\vec{G} + \vec{k}f) \cdot (\vec{G} + \vec{k}f)^*) e^{-t(\frac{1}{2}+\gamma)} dt \\ \Psi_{\vec{u}}(f, \gamma) &= \vec{p} - \text{Tr}[\gamma \vec{k}] - f^* \vec{k} f - 2\text{Re}(f^* \vec{G}) \end{aligned}$$

defined on balls of centers $0, 0, 0, \frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{p}$ and \vec{p} and proving that the application

$$\Psi_{(f,\lambda)}(f, \lambda) = (\Psi_f[f, \Psi_\alpha\{f, \lambda\}], \Psi_\gamma\{\Psi_\alpha(f, \lambda)\}, \Psi_{\vec{u}}\{f, \Psi_\gamma(\Psi_\alpha[f, \lambda])\}], \\ \Psi_\lambda[f, \Psi_\gamma\{\Psi_\alpha(f, \lambda)\}], \Psi_{\vec{u}}\{f, \Psi_\gamma(\Psi_\alpha[f, \lambda])\}])$$

is a contraction for a convenient choice of the radiuses and a sufficiently small coupling constant g . Note that it is then convenient to consider the norm of $L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2, |\vec{k}|^2)$ for f .

Proof of Theorem VIII.1. Indeed, set $\vec{u} = \vec{p} - \text{Tr}[\gamma\vec{k}] - f^*\vec{k}f - 2\text{Re}(f^*\vec{G})$ and define the partial derivatives as $\partial_{f^*}\mathcal{E}(f, \gamma, \alpha) \in \mathcal{Z}$, $\partial_{\alpha^*}\mathcal{E}(f, \gamma, \alpha) \in \mathcal{Z}^{\vee 2}$ and $\partial_\gamma\mathcal{E}(f, \gamma, \alpha) \in \mathcal{B}(\mathcal{Z}) \cong \mathcal{L}^1(\mathcal{Z})'$ such that

$$\begin{aligned} \mathcal{E}(f + \delta f, \gamma + \delta\gamma, \alpha + \delta\alpha) - \mathcal{E}(f, \gamma, \alpha) \\ = 2\text{Re}(\delta f^* \partial_{f^*}\mathcal{E}(f, \gamma, \alpha)) + 2\text{Re}(\delta\alpha^* \partial_{\alpha^*}\mathcal{E}(f, \gamma, \alpha)) \\ + \text{Tr}[\delta\gamma \partial_\gamma\mathcal{E}(f, \gamma, \alpha)] + o(\|(\delta f, \delta\gamma, \delta\alpha)\|_{\mathcal{Z} \times \mathcal{L}^1(\mathcal{Z}) \times \mathcal{Z}^{\vee 2}}). \end{aligned}$$

Recall the energy functional is given by Equation (IV.62) and this yields

$$\begin{aligned} \partial_{f^*}\mathcal{E}(f, \gamma, \alpha) &= \frac{1}{2}\{2(\vec{k}f + \vec{G}) \cdot (\text{Tr}[\gamma\vec{k}] + f^*\vec{k}f + 2\text{Re}(f^*\vec{G}) - \vec{p}) \\ &\quad + 2\vec{k} \cdot \vee(\vec{G} + \vec{k}f)^*\alpha + \vec{k} \cdot (2\gamma + \mathbf{1})(\vec{G} + \vec{k}f)\} + |\vec{k}|f \\ &= -(\vec{k}f + \vec{G}) \cdot \vec{u} + \vec{k} \cdot \vee(\vec{G} + \vec{k}f)^*\alpha + \vec{k} \cdot (\gamma + \frac{1}{2}\mathbf{1})(\vec{G} + \vec{k}f) + |\vec{k}|f \\ &= M(\gamma, \vec{u})f + (\vec{k}(\gamma + \frac{1}{2}\mathbf{1}) - \vec{u}) \cdot \vec{G} + \vec{k} \cdot \vee(\vec{G} + \vec{k}f)^*\alpha, \\ \partial_{\alpha^*}\mathcal{E}(f, \gamma, \alpha) &= \frac{1}{2}(\vec{k} \cdot \otimes \vec{k})\alpha + \frac{1}{2}(\vec{G} + \vec{k}f)^{\vee 2}, \\ \partial_\gamma\mathcal{E}(f, \gamma, \alpha) &= \frac{1}{2}\{2\vec{k} \cdot (\text{Tr}[\gamma\vec{k}] + f^*\vec{k}f + 2\text{Re}(f^*\vec{G}) - \vec{p}) \\ &\quad + 2\vec{k} \cdot \gamma\vec{k} + |\vec{k}|^2 + 2(\vec{G} + \vec{k}f) \cdot (\vec{G} + \vec{k}f)^*\} + |\vec{k}| \\ &= M(\gamma, \vec{u}) + (\vec{G} + \vec{k}f) \cdot (\vec{G} + \vec{k}f)^*. \end{aligned}$$

The constraint given by Equation (III.60) can be expressed as

$$\mathcal{C}(f, \gamma, \alpha) = 0 \tag{VIII.75}$$

with

$$\begin{aligned} \mathcal{C} : \mathcal{Z} \times \mathcal{L}^1(\mathcal{Z}) \times \mathcal{Z}^{\vee 2} &\rightarrow \mathcal{L}^1(\mathcal{Z}) \\ (f, \gamma, \alpha) &\mapsto \gamma + \gamma^2 - (\alpha^* \otimes \mathbf{1}_{\mathcal{Z}})(\mathbf{1}_{\mathcal{Z}} \otimes \alpha). \end{aligned}$$

Equation (VIII.75) is equivalent to Equation (VIII.72). The application \mathcal{C} has a differential $DC(f, \gamma, \alpha) : \mathcal{Z} \times \mathcal{L}^1(\mathcal{Z}) \times \mathcal{Z}^{\vee 2} \rightarrow \mathcal{L}^1(\mathcal{Z})$ such that

$$DC(f, \gamma, \alpha)(\delta f, \delta \gamma, \delta \alpha) \\ = \delta \gamma + \delta \gamma \gamma + \gamma \delta \gamma - (\delta \alpha^* \otimes \mathbf{1}_{\mathcal{Z}})(\mathbf{1}_{\mathcal{Z}} \otimes \alpha) - (\alpha^* \otimes \mathbf{1}_{\mathcal{Z}})(\mathbf{1}_{\mathcal{Z}} \otimes \delta \alpha).$$

For $\|\gamma\|_{\mathcal{B}(\mathcal{Z})} < \frac{1}{2}$ the application $DC(f, \gamma, \alpha)$ is surjective. Indeed it is already surjective on $\{0\} \times \mathcal{L}^1(\mathcal{Z}) \times \{0\}$, since, for every $\gamma' \in \mathcal{L}^1(\mathcal{Z})$ the equation $\delta \gamma + \delta \gamma \gamma + \gamma \delta \gamma = \gamma'$ with unknown $\delta \gamma$ has at least one solution, see Proposition VIII.3. We can then apply the Lagrange multiplier rule (see for example the book of Zeidler [10]) which tells us that there exists a $\lambda \in \mathcal{B}(\mathcal{Z})$ such that

$$\forall(\delta f, \delta \alpha, \delta \gamma), \quad D\mathcal{E}(f, \alpha, \gamma)(\delta f, \delta \alpha, \delta \gamma) + \text{Tr}[DC(f, \alpha, \gamma)(\delta f, \delta \alpha, \delta \gamma) \lambda] = 0,$$

that is to say

$$2\text{Re}(\delta f^* \partial_{f^*} \mathcal{E}(f, \gamma, \alpha) + \delta \alpha^* \partial_{\alpha^*} \mathcal{E}(f, \gamma, \alpha)) + \text{Tr}[\partial_{\gamma} \mathcal{E}(f, \gamma, \alpha) \delta \gamma] \\ + \text{Tr}[(\delta \gamma + \delta \gamma \gamma + \gamma \delta \gamma - (\delta \alpha^* \otimes \mathbf{1}_{\mathcal{Z}})(\mathbf{1}_{\mathcal{Z}} \otimes \alpha) - (\alpha^* \otimes \mathbf{1}_{\mathcal{Z}})(\mathbf{1}_{\mathcal{Z}} \otimes \delta \alpha)) \lambda] = 0.$$

This is equivalent to Equations (VIII.70), (VIII.71) and

$$\lambda(\frac{1}{2} + \gamma) + (\frac{1}{2} + \gamma)\lambda = M(\gamma, \vec{u}) + (\vec{G} + \vec{k}f) \cdot (\vec{G} + \vec{k}f)^* \quad (\text{VIII.76})$$

Using again Proposition VIII.3 we get that Equation (VIII.76) is equivalent to Equation (VIII.73).

For the invertibility of $\mathcal{A}(\lambda)$ note that

$$\mathcal{A}(\lambda) = \frac{1}{4}(\vec{k} \otimes \mathbf{1} + \mathbf{1} \otimes \vec{k})^2 + (|\vec{k}| - \vec{k} \cdot \vec{p} + \lambda - \frac{1}{2}|\vec{k}|^2 - |\vec{k}| + \vec{k} \cdot \vec{p}) \vee \mathbf{1} \\ \geq (\frac{\sigma}{2} - \lambda - (|\vec{k}|^2/2 + |\vec{k}| - \vec{p} \cdot \vec{k})\|_{\mathcal{B}}) \mathbf{1} \vee \mathbf{1}.$$

For $M(\gamma, \vec{u})$, $M(\gamma, \vec{u}) = \frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u} + \vec{k} \cdot \gamma \vec{k} \geq \sigma/2$ if $\gamma \geq 0$ and $|\vec{u}| < 1/2$. \square

Let us recall a well known expression for the solution of the Sylvester or Lyapunov equation.

Proposition VIII.3. *Let A and B be bounded self-adjoint operators on a Hilbert space. Suppose $A \geq a \mathbf{1}$ with $a > 0$. Then the equation*

$$AX + XA = B$$

for X a bounded operator has a unique solution $\chi_A(B) = \int_0^\infty e^{-tA} B e^{-tA} dt$. If B a trace class operator then the solution X is also trace class.

Proof. Indeed, $\chi_A(B)$ is a solution because

$$\begin{aligned} A\chi_A(B) + \chi_A(B)A &= \int_0^\infty e^{-tA}(AB + BA)e^{-tA}dt \\ &= - \int_0^\infty \frac{d}{dt}(e^{-tA}Be^{-tA})dt = B. \end{aligned}$$

Conversely, suppose that $AX + XA = B$, then

$$\begin{aligned} \chi_A(B) &= \int_0^\infty e^{-tA}(AX + XA)e^{-tA}dt \\ &= - \int_0^\infty \frac{d}{dt}(e^{-tA}Xe^{-tA})dt = X, \end{aligned}$$

and thus any solution X is equal to $\chi_A(B)$. Hence the solution is unique. \square

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